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SELECTION AND APPLICATION OF AN URBAN AIR QUALITY MODEL FOR ALBERTA

RESEARCH MANAGEMENT DIVISION

Alberta Environment

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SELECTION AND APPLICATION OF AN URBAN AIR QUALITY MODEL FOR ALBERTA

by

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Concord Scientific Corporation

for

RESEARCH MANAGEMENT DIVISION
Alberta Environment

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EXECUTIVE SUMMARY

The quality of air in an urban environment is dependent on many factors. Pollutant emissions, background air quality, atmospheric chemistry, atmospheric transport, and deposition interact in very complex ways. The best way currently available to quantify the important processes and their interactions is to make use of a mathematical model. Such models simulate the important processes which occur in the urban atmosphere and permit an assessment of both the impact due to emissions from a given source or group of sources, and the effectiveness of various levels of control on such sources.

Major urban centres (Edmonton and Calgary) are prone to high pollutant levels or episodes. Historical records have shown frequent violations of the ozone air quality objectives in Edmonton and Calgary. Continued urban growth will result in even more frequent observation of high ambient concentrations of pollutants. Improvements in air quality (or the prevention of deterioration of air quality requires that emissions be controlled. The most efficient and cost-effective method of designing such control measures is to make use of a mathematical air quality model, which provides a direct and quantitative link between emissions and pollutant concentrations.

The Research Management Division of Alberta Environment contracted Concord Scientific Corporation to review urban air quality models for application to major urban centres in Alberta. Specifically, the study objectives were:

1. To identify and evaluate available urban air quality simulation models with respect to the adequacy of their treatment of the quantitative relationships between urban emissions, background air quality, ambient pollutant concentrations, atmospheric dispersion, chemical transformations, removal processes, and probable effects;
2. To make recommendations pertaining to the suitability and applicability of the models to Alberta's major urban centres given existing monitoring networks and objectives.

Forty-two models were identified initially. Initial screening criteria were established based upon the needs and requirements of Alberta Environment. The initial criteria were:

1. Three dimensional, Eulerian formulation;
2. Detailed photochemical mechanism; and
3. Availability of detailed model descriptions.

Application of the initial screening criteria to the original list of models resulted in the retention of four models which were carried forward for detailed evaluation. The four models were LIRAQ, Urban Airshed Model, McRae et al., and IMPACT.

The selection process was based on a detailed, component by component examination of the models, and employed the following criteria:

1. Completeness of model;
2. Basic scientific soundness of the treatment of each process;
3. Balance of the components within the model; and
4. Accessibility.

The Urban Airshed Model emerged as the superior model. Detailed investigation of comparison and sensitivity studies performed with UAM provided further confirmation of its credibility as an air quality prediction tool. Examination of the running requirements of UAM showed that it is flexible in the quantity and quality of data required. It could be run with the existing data available in Alberta.

The recommendations resulting from this work are:

1. The Urban Airshed Model should be implemented for application to the study of air quality in urban centres in Alberta.
2. The model should be exercised using its minimum input options to allow experience to be gained in its operation.
3. Plans should be prepared for programs that will provide the input and validation data necessary for the production of credible model predictions.
4. A wind field generator should be selected/developed which would incorporate some of the site specific features of Alberta.

5. The following model refinements should be considered:
   i) The most up-to-date version of CBM should be installed;
   ii) Introduce state-of-the-art numerical procedures to reduce the amount of false diffusion introduced by the transport algorithm; and
   iii) Use implicit formulations and vectorization to reduce computational effort.

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ABSTRACT

The need to monitor existing and future air quality in the major urban centres in Alberta prompted Alberta Environment to sponsor Concord Scientific Corporation to review urban air quality models. The objectives were to identify and evaluate available urban air quality simulation models and to make recommendations pertaining to the suitability and applicability of the models to Alberta's major urban centres. Of the the 42 models initially identified, the three dimensional, Eulerian Urban Airshed Model was selected as best suited to the needs of Alberta Environment. The structure of the UAM is such that it could be applied to urban centres in Alberta given the existing databases. It is recommended, however, that programs be prepared that will provide a more extensive input and validation database, and a state-of-the-art chemical mechanism and numerical solution scheme be implemented.

ACKNOWLEDGEMENTS

Grateful acknowledgement is given to the Research Management Division of Alberta Environment for their sponsorship of this study. Particular thanks is given to Ms. Bonnie Magill, Research Manager at Alberta Environment for her efforts in providing Concord Scientific with information on existing air quality networks in Alberta.

1. INTRODUCTION

Calgary and Edmonton, the two major urban centres in Alberta, have air quality monitoring networks that measure ambient levels of total suspended particulates (TSP), carbon monoxide (CO), nitrogen dioxide (NO_2), sulphur dioxide (SO_2), ozone (O_3), soiling index (COH) and total dustfall. The networks in each city are operated by the Alberta Government's Pollution Control Division but include stations reported in the federally operated National Air Pollution Surveillance (NAPS) network. Data are also available from a network operated by the Strathcona Industrial Society, which monitors air quality in the industrial district on the outskirts of Edmonton. Data from these networks are summarized each year in annual reports (Air Monitoring Report, Edmonton Metropolitan Area; Air Monitoring Report, City of Calgary; Annual Summary, National Air Pollution Surveillance Network). Annual Reports for the Edmonton Metropolitan Area and for Calgary are available up to 1979.

Comparison of the reported pollutant levels with provincial air quality standards or federal air quality objectives to determine the frequency with which these standards or objectives are exceeded allows a rapid assessment of the air quality in the two cities. This information is contained in the annual reports referenced above. Other assessments of air quality in these cities have been published from time to time, based on special studies in which additional pollutants were monitored (e.g., Peake et al. 1983; Peake and Sandhu 1983; Sandhu 1975; Nkemdirim 1976) or on consolidated analyses of historical data (e.g., CSC 1984; Ricci 1979).

Examination of historical data shows that in Edmonton, for example, there have been no violations of the provincial standards for SO_2 (1-hour or 24-hour average). In the cases of NO_2, O_3, CO, and TSP, however, there have been a number of occasions on which provincial standards or federal air quality objectives have been exceeded (see Table 1 for a summary of such data for the years 1977

to 1983). Similar data for Calgary, also based on comparison with Federal air quality objectives, are given in Table 2.

The observation of frequent violations of the ozone air quality objectives in both cities is especially important given their northern latitude and the concomitant (relatively) low amounts of sunlight available for photochemical reactions. In Edmonton, for example (CSC 1982), the high levels of total hydrocarbons and moderate levels of nitrogen dioxide provide some basis for explaining the observed high levels of ozone and other secondary pollutants. Furthermore, the urban plume from Edmonton is likely to be significant in affecting air quality (e.g., ozone levels: Peake et al. 1983) downwind of the city. In Calgary, levels of peroxyacetylnitrate (PAN) as high as 2.4 ppb in west Calgary and 6.6 ppb in downtown Calgary have been reported (Peake et al. 1983).

It is thus clear from the historical record that high pollutant levels have been observed in both cities. It is to be expected that urban growth will continue, leading to increased emissions of primary pollutants, such as carbon monoxide, the oxides of nitrogen and volatile organic compounds, and resulting in more frequent observation of high ambient concentrations of pollutants. Improvements in air quality (or the prevention of deterioration of air quality) requires that emissions be controlled. The most efficient and cost effective method of designing such control measures is to make use of a mathematical air quality model, which provides a direct and quantitative link between emissions and pollutant concentrations.

The study described in this report was therefore carried out under contract to the Research Management Division of Alberta Environment. The study objectives were:

1. To identify and evaluate available urban air quality simulation models (UAQSM's) with respect to the adequacy of their treatment of the quantitative relationships between urban emissions, background air quality, ambient pollutant concentrations, atmospheric dispersion, chemical transformations, removal

Table 1. Number of readings in excess of federal air quality objectives[a] for City of Edmonton, 1977 to 1983.

Pollutant and Averaging Period	Federal Air Quality Objectives[b]		Number of Readings in Excess of Federal Air Quality Objectives and Number of Stations (x)						
			1983	1982	1981	1980	1979	1978	1977[e]
Nitrogen Dioxide									
1-h average	0.21	A[c]	0(2)	2(2)	1(3)	2(2)	0(2)	0(2)	0(3)
24-h moving average	0.11	A	24(2)	50(2)	0(3)	0(2)	0(2)	0(2)	0(3)
Ozone									
1-h average	0.05	D[d]	275(2)	602(2)	350(2)	168(2)	356(2)	104(2)	98(3)
24-h moving average	0.015	D	7610(2)	8706(2)	7306(2)	6101(2)	6919(2)	5283(2)	412(3)
Carbon Monoxide									
1-h average	13.0	D	32(3)	29(3)	60(3)	42(3)	81(3)	26(3)	39(3)
8-h moving average	5.0	D	379(3)	475(3)	632(3)	1143(3)	1614(3)	543(3)	84(3)
Sulphur Dioxide									
1-h average	0.17	D	0(1)	0(1)	0(3)	0(3)	0(3)	0(3)	0(3)
24-h moving average	0.06	D	0(1)	0(1)	0(3)	0(3)	0(3)	0(3)	0(3)
Total Suspended Particulates	120	A	13(3)	26(3)	37(3)	54(4)	68(5)	46(5)	78(5)

a Data extracted from NAPS annual summaries 1978 to 1983, and from 1977 air monitoring reports, City of Edmonton.

b All values in ppm except for Total Suspended Particulates (TSP), which is in $\mu g/m^3$. Note these federal air quality objectives are identical to the Alberta provincial air quality standards for all pollutants except TSP. The provincial standard for TSP is 100 $\mu g/m^3$.

c A-Maximum Acceptable Level

d D-Maximum Desirable Level

e Daily average (i.e., not moving average) used to calculate number of readings exceeding 24-hour provincial standards.

Table 2. Number of readings in excess of federal air quality objectives[a] for City of Calgary, 1977 to 1983.

Pollutant and Averaging Period	Federal Air Quality Objectives[b]		Number of Readings in Excess of Federal Air Quality Objectives and Number of Stations (x)						
			1983	1982	1981	1980	1979	1978	1977[e]
Nitrogen Dioxide									
1-h average	0.21	A[c]	2(2)	1(2)	0(2)	5(2)	10(3)	9(2)	18(3)
24-h moving average	0.11	A	0(2)	28(2)	0(2)	15(2)	59(3)	134(2)	10(3)
Ozone									
1-h average	0.05	D[d]	197(2)	453(2)	207(2)	249(2)	593(3)	232(2)	363(3)
24-h moving average	0.015	D	8234(2)	8646(2)	7428(2)	8226(2)	8041(3)	8928(2)	446(3)
Carbon Monoxide									
1-h average	13.0	D	66(3)	38(2)	69(2)	79(2)	87(3)	74(2)	103(3)
8-h moving average	5.0	D	498(3)	367(2)	576(2)	577(2)	803(3)	800(2)	129(3)
Sulphur Dioxide									
1-h average	0.17	D	0(1)	0(3)	0(3)	0(3)	0(4)	0(3)	0(3)
24-h moving average	0.06	D	0(1)	0(3)	0(3)	0(3)	0(4)	0(3)	0(3)
Total Suspended Particulates	120.0	A	35(3)	54(3)	78(3)	96(4)	75(4)	56(4)	60(4)

a Data extracted from NAPS annual summaries 1978 to 1983, and from 1977 air monitoring reports, City of Calgary.

b All values in ppm except for Total Suspended Particulates (TSP), which is in $\mu g/m^3$. Note these federal air quality objectives are identical to the Alberta provincial air quality standards for all pollutants except TSP. The provincial standard for TSP is 100 $\mu g/m^3$.

c A-Maximum Acceptable Level

d D-Maximum Desirable Level

e Daily average (i.e., not moving average) used to calculate number of readings exceeding 24-hour Provincial standards.

processes, and probable effects. The selection process was not restricted necessarily to a single model; the possibility of integrating components from two or more models was also considered.

2. To make recommendations pertaining to the suitability and applicability of the models to Alberta's major urban centres given existing monitoring networks and objectives. The adequacy of the existing monitoring networks and emissions inventories was assessed. Based on the model(s) selected, research and monitoring programs to provide data specific to the requirements of the model(s) have been outlined.

As will be described in Section 3, it was determined that a model of the Eulerian type would be most suitable for application to urban centres in Alberta. An overview of urban scale modelling, with particular reference to Eulerian models, is given in Section 2. Preliminary screening of the models, and a detailed discussion of those surviving the screening, are contained in Section 3, together with the selection of the model felt to be best for the proposed application. The data input and hardware requirements of the selected model are described in Section 4, while Section 5 gives a brief summary of models which might be used to investigate purely local effects (e.g., street canyon), and those that describe the impact of the urban plume at downwind points. The conclusions and recommendations are presented in Sections 6 and 7 respectively.

2. OVERVIEW OF URBAN MODELLING

The dynamic behaviour of air pollutants in an urban environment is dependent on the interactions between the meteorology, including wind speed and direction, inversion height and atmospheric stability, the source emissions, and the kinetic mechanism for atmospheric chemical reactions among pollutant species at the particular time and location of interest. An effective pollution control strategy requires a model of these physical phenomena and their interactions, that will provide a quantitative relationship between source emissions and the resulting ambient air quality levels.

The most common and useful way of relating the above phenomena is to express them in a transport equation describing the mass conservation of the pollutant species in a turbulent fluid in which chemical reactions occur. This equation can be written in the following manner:

$$\underset{(I)}{\frac{\partial C_i}{\partial t}} + \underset{(II)}{\frac{\partial}{\partial x} uC_i + \frac{\partial}{\partial y} vC_i + \frac{\partial}{\partial z} wC_i} = \underset{(III)}{\frac{\partial}{\partial x}\left(\overline{-u'c_i'}\right) + \frac{\partial}{\partial y}\left(\overline{-v'c_i'}\right) + \frac{\partial}{\partial z}\left(\overline{-w'c_i'}\right)} + \underset{(IV)}{S} \quad , \qquad \text{Equation 1}$$

where C_i represents the pollutant concentration and is a function of space (x,y,z) and time (t). The wind field components (u,v,w) correspond to the three spatial directions.

This equation expresses the rate of change of pollutant concentration (I) due to transport (advection) by the mean wind field (u,v,w) (II), diffusion by turbulence ($\overline{-u'c'}$, $\overline{-v'c'}$, $\overline{-w'c'}$) (III), and by sources and sinks of the pollutant (IV). Term IV will contain terms for emission sources, chemical reactions, and wet and dry deposition. In this report, advection refers to transport by the mean wind in the two horizontal directions (u,v), and convection refers to transport in the vertical direction.

In deriving the continuity equation three assumptions were necessary: first, that effects due to molecular diffusion are small

relative to those attributable to turbulent diffusion; second, that pollutant transport due to turbulence can be adequately represented by partitioning the turbulent field into a slowly varying mean field with a rapidly fluctuating turbulent field superimposed; and third, that turbulent concentration fluctuations have a negligible influence on reaction rates. A thorough discussion of the derivation of the continuity equation can be found in McRae et al. (1982a).

With the specification of appropriate boundary and initial conditions, solution of the transport equations will give the temporal and spatial variation of the pollutants. Unfortunately, the resulting set of equations is non-linear, coupled (through the source parameters and sink terms), and in its current form, has more unknowns than equations. It is necessary to introduce parametrizations to make the equations tractable, and either to simplify the equations, thus limiting their applicability, or to retain their full three-dimensional, transient form and choose a numerical procedure to solve them.

Solution of the complete mass conservation equation poses many problems. Traditional approaches have generally simplified the equation by focusing only on the terms applicable to a particular problem. For example, a point source emitter of inert species in steady state can be solved analytically in a Gaussian model. Alternatively, if transport and diffusion are ignored, leaving only the first and last terms in Equation 1, a box model results, in which the airshed is simulated like a smog chamber. However, because most urban airsheds are topographically and meteorologically complex, such broad assumptions are generally not acceptable.

In this report attention is devoted to Eulerian models; this restriction is discussed further in Section 3. An Eulerian model retains the original form of the mass conservation equation, and applies assumptions on how the concentration varies spatially and temporally, such that a solution is obtained in a grid that covers the airshed. The equation is only altered to reflect the averaging required for use in a numerical model with finite space and time increments. The major advantage of Eulerian models is that

they allow for a complete solution of pollutant concentrations at all points in the airshed at each time step.

Developing and implementing an Eulerian model is a difficult undertaking because it is necessary to maintain a balance between the need for computational economy and the desire for an accurate representation of the underlying physics and chemistry. In the following sections the major assumptions and parametrizations typically used in three-dimensional (Eulerian) urban air quality models will be discussed. The topics discussed are transport and diffusion (Terms II and III of Equation 1), sources and sinks (Term IV), and the numerical methods employed to solve the equations.

2.1 TRANSPORT AND DIFFUSION

Important factors in calculating transport and diffusion are the treatment of atmospheric turbulence and the specification of the mean wind field.

2.1.1 Turbulence Closure

In deriving the general, turbulent continuity equation it was assumed that the effects of turbulence can be modelled by representing the field variables as the sum of a mean and a fluctuating component. For example, a general variable ϕ (e.g., a wind vector component) is expressed as:

$$\phi = \bar{\phi} + \phi' \quad , \qquad \text{Equation 2}$$

where the overbar represents the mean value, and the prime the fluctuating component. Substituting Equation 2 into the general continuity equation, and time averaging to get the average effects resulting from the turbulent motion, produces the turbulent concentration fluxes $-\overline{u'c'}$, $-\overline{v'c'}$, and $-\overline{w'c'}$. Solution of the continuity equation requires knowledge of the spatial variation of these fluxes throughout the solution domain, and also knowledge of how they vary in response to different meteorological and topographical conditions.

Very complex turbulence models have been developed for this purpose. The most complex are higher order schemes that solve

conservation equations for the turbulent correlation terms themselves. These models have been used primarily to close the momentum equations in planetary boundary layer wind field models (e.g., Wyngaard et al. 1974). The results can be related to concentration fluxes through a constant that relates mass and momentum transfer.

The highest degree of physical realism is provided in this type of closure as it allows direct incorporation of the relevant meteorological influences, i.e., heating and cooling at the earth's surface. Unfortunately the non-linear nature of these equations makes their use computationally prohibitive.

A more common approach taken in air quality modelling is to relate the turbulent fluxes to the mean variables in the continuity equation rather than to solve for the fluxes themselves. This approach, known as K theory, is based on an analogy between molecular and turbulent diffusion. It is assumed that the turbulent fluxes are equal to the product of a flow-dependent turbulent diffusivity K, and the mean concentration gradient.

$$-\overline{u'c'} = K_x \frac{\partial \bar{c}_i}{\partial x} \qquad \text{Equation 3}$$

$$-\overline{v'c'} = K_y \frac{\partial \bar{c}_i}{\partial y}$$

$$-\overline{w'c'} = K_z \frac{\partial \bar{c}_i}{\partial z}$$

It is important to note that the turbulent viscosities are not constant, measured, fluid properties like the molecular viscosity, but are dependent on the turbulent nature of the flow. It is therefore still necessary either to solve further equations for turbulent properties that can be used to characterize the turbulent diffusivity, or to specify the diffusivity, using experimental data or higher order numerical results that have taken into account the relevant meteorological conditions.

An example of a turbulent model of the former type would be the turbulent kinetic energy - dissipation rate of turbulent kinetic energy (k-e) model. In this model (Launder and Spalding 1974) conservation equations are solved for the kinetic energy and dissipa-

tion rate of the turbulence. These two quantities are combined to give characteristic turbulent velocity and length scales, which in turn can be combined to give the turbulent viscosity. The turbulent viscosity must then be related to the turbulent diffusivity by use of a characteristic turbulent Prandtl number.

Two-equation K theory models are much less cumbersome computationally than the higher order closures, and can still incorporate much of the relevant physics, though in a more empirical fashion. But again, the added computational cost makes their use in a three-dimensional model impractical.

Because of computational restrictions, the closure used in each of the models reviewed in this report is the specification of the diffusivity as a function of space and local meteorological and topographical conditions.

The specified variation of the diffusivity is very important, especially in the vertical direction, as this must be used to account for the process of entrainment from above the inversion. Vertical diffusivity profiles handle this by gradually reducing to a small value at the top of the mixed layer, and then maintaining a small value in the stable layer above the inversion. Horizontal diffusion is often negligible relative to horizontal advection (Reynolds et al. 1973; McRae et al. 1982a). Horizontal diffusivity are therefore commonly set to small constant values.

The limitations of specified K, and K theory in general, are well documented, and are considered to be a major potential source of invalidity in Eulerian models. However, at the present time computational limitations preclude the use of the higher order closures. As long as the viscosity functions used in the model have been determined empirically under conditions similar to those to which the equation is applied, then the approximation may be considered valid.

2.1.2 Wind Field

An important, and at many times dominant factor in determining the pollutant concentration over an urban area is the

advection of the pollutant by the mean wind field. Therefore, a key input to an urban-scale air pollution model is an accurately specified, mass consistent wind field. The greatest amount of physical realism and control strategy flexibility can be obtained by solving the full, three-dimensional, Navier-Stokes equations together with the various species conservation equations. Unfortunately, in most practical situations, numerical solution of the full Navier-Stokes equations is not feasible as a means of constructing such a field. It is also impractical to attempt to observe winds with the spatial and temporal resolution required for input to the dispersion model. It is therefore necessary to assume that the presence of pollutant gases and particulates does not significantly affect meteorology. This assumption effectively decouples the velocity and temperature fields from the species conservation equations, thus allowing the velocity and temperature fields to be supplied by a more computationally efficient method.

The most common approach for generating a gridded wind field is to use objective analysis techniques that have as their basis the (generally limited) meteorological data for the area of interest. These methods consist of two basic steps. The first is to interpolate the sparse and discrete surface and, if available, upper air data onto the chosen three-dimensional grid. Once the initial field has been established, the next step is to employ an objective analysis procedure to adjust the wind vectors at each grid point so that an appropriate physical constraint is satisfied. A common choice is the conservation of mass.

It is of considerable importance that the final wind field satisfy the conservation of mass. If it does not, then the mass gained or lost in a grid volume can invalidate any calculated transport or diffusion of air pollution.

If the air quality model is to be run in an area where there is very complex topography and/or active and changing meteorological processes, it is necessary that the wind field generation routine respond by channelling and diverting the flow field in these areas.

Other characteristics that must be considered in evaluating these wind field models is whether they include effects of local surface roughness and stability, whether they can be used for the specification of initial concentration and temperature fields, whether they require any empirical constants, and the nature of their input data requirements. A point tied into the input data requirements is whether the model allows the boundary values to adjust with the internal field, or requires them to be kept fixed. Adequate data is necessary for the effective use of these models. The appropriateness of the data is dependent on the grid size used. For example, if the grid square size is 10 km by 10 km, then the wind data should be sufficient to allow estimation of a wind network with an average spacing of approximately 10 km. As an example, McRae and Seinfeld (1983) used 63 surface wind stations and 6 upper air stations to generate the wind field for an 80 by 32 array of grid squares, each 5 km by 5 km.

Interpolation and adjustment schemes have major programming and computational requirements. However, when compared with the requirements of numerical solution of the Navier-Stokes equations, or the impracticality of making observations at a resolution high enough for these models, they are, at present, the best way to generate wind fields for dispersion models, as long as adequate data are available.

2.2 SOURCES AND SINKS

Sources and sinks of pollutant species in an urban environment include (as sources), point, area, and volume emissions from stacks, traffic, etc., and (as sinks), wet and dry deposition by rainfall or surface interaction. Chemical reactions can constitute both sources and sinks. Atmospheric chemistry is of considerable importance in urban air quality modelling. Ozone, for example, is not emitted directly, but is produced by chemical reaction. Because of its unique characteristics, chemistry will be discussed separately in Section 2.2.1. Attention will be given here to the treatment of emission and removal processes.

The first step in dealing with sources for an urban air quality model requires taking an actual inventory of source emissions for the particular area of interest. This includes, for example, fixed source emissions and automotive and aircraft emissions (Roth et al. 1974). While it is perhaps the most tedious and mundane aspect of urban airshed modelling, it is of utmost importance in model validation. If done properly, it probably constitutes the most precise segment of the requisite input data. It is therefore essential to devote considerable effort to the establishment of an accurate emissions inventory for the region to be modelled. Consideration must also be given to the requirements for spatial, temporal, and chemical resolution that are imposed on the emission inventory by the model. These requirements have been reviewed recently (CSC 1984a) as the initial step in designing an emission inventory for Vancouver.

The detail required in the emission inventory is determined to a great extent by the region being considered and by a realistic assessment of the prediction capabilities of the model. Emphasis should be given to those sources that have the greatest regional effect, but attention should also be given to sources that, while responsible for only a small portion of the total emissions on a regional basis, contribute substantially to pollutant levels in their own locale.

Following the collection of the emissions data, it is necessary to represent the data mathematically in an accurate and realistic way for use in the model. The key to this representation is in the resolution of the basic incompatibility between point sources/measurements and urban-scale model predictions for grid squares of the order of square kilometres. One method of dealing with this problem is to develop sub-grid scale models that predict the local influences of localized sources. Examples of these would be highway and street canyon models, which are discussed in Section 5. Despite the diversity of different source types, pollutants and models of material discharge, most emissions can be considered to be released from either point locations or areal regions.

In dealing with fixed sources (stacks), all that is required in the emissions inventory is accurate information on mass emissions from each important fixed source in the area. If the source is considered to be a ground source, then it can be included in the boundary conditions. For elevated sources (embedded plumes) the most common allocation scheme is to add the emissions from the source into the grid cell at the effective stack height. If all the material is injected into one cell, the near source air quality impact can be overestimated. Particular problems may also arise when non-linear processes take place, e.g., chemical reactions. It is therefore important that dispersion of the plume be accounted for in some realistic way. In particular, allowing the emissions to be dispersed downwind, taking into account the actual vertical and lateral spread of the plume, as well as determining whether the effective stack height is above or below the top of the mixed layer, will provide a more realistic prediction.

Pollutants are removed from the air by deposition processes such as adsorption of gases to surfaces, fallout of heavy particulates, and washout of gases and particulates by precipitation processes. Deposition processes are difficult to quantify in complex flow, and the process is therefore parametrized in an approximate way.

In general, the dry deposition rate is assumed to be proportional to the concentration in the layer closest to the surface or to some implied surface concentration. The constant of proportionality is called the deposition velocity, v_g. Ideally, the deposition velocity will account for the complex linkage between the turbulent diffusion in the surface layer, the molecular interaction of the air-ground interface, and the chemical interaction of the pollutant with the surface. Because of the difficulty in doing this, the deposition velocity for a chemical species is often specified to be a constant, its value being determined from experimental results. Other workers have given a more comprehensive treatment to the calculation of deposition velocities by modelling them in terms of an

electrical resistance analog. This treatment permits the value to be related to atmospheric and surface parameters.

The estimation of wet deposition is, in some ways, more difficult than dry deposition. This is because precipitation, the mechanism that drives wet deposition, is intermittent in time, space, and intensity, whereas the factors that influence dry deposition are relatively constant. The response of the pollutant being carried by the air to precipitation depends on many complex factors, which are only partially understood. None of the models being reviewed in this report treats wet deposition, since the formation of urban pollutants of major concern (O_3, PAN) is driven by sunlight. Therefore, wet deposition will, not be discussed further here.

2.2.1 Urban Atmospheric Chemistry

Detailed mechanisms of atmospheric photochemistry, including the reactions of organic species, have been published by a number of authors (e.g., Demerjian et al. 1974; Derwent and Hov 1980; Falls and Seinfeld 1978; Lloyd 1978; Graedel et al. 1976). The species generally of concern in the atmosphere include ozone, oxides of nitrogen, nitric and sulphuric acids, and peroxyacetyl nitrate (PAN). Air quality monitoring data for Calgary and Edmonton indicate that high levels of ozone, nitrogen dioxide, and total hydrocarbons occur in these cities (e.g., Alberta Environment 1981, 1982).

Ozone formation is generally initiated by the photolysis of NO_2, followed by reaction of the resulting oxygen atom with an oxygen molecule:

$$NO_2 + h\nu \rightarrow NO + O \quad , \qquad \text{Equation 4}$$

$$O + O_2 \rightarrow O_3 \quad . \qquad \text{Equation 5}$$

The reverse reaction also occurs,

$$NO + O_3 \rightarrow NO_2 + O_2 \quad , \qquad \text{Equation 6}$$

and a stationary state may be reached where the net rates of the forward and reverse reactions are equal, i.e.,

$$k_1 [NO_2] = k_2 [NO] [O_3] \quad . \qquad \text{Equation 7}$$

$$\text{Therefore} \qquad [O_3] = \frac{k_1[NO_2]}{k_2 [NO]} \quad . \qquad \text{Equation 8}$$

The reaction in Equation 5 is very rapid and is assumed to occur virtually instantaneously.)

The implication of Equation 8 is that any process that enhances conversion of NO to NO_2 will produce an enhancement of ozone production.

In fact, this conclusion remains valid even if the stationary state is not achieved, since the next rate of ozone production is given by ($k_1 [NO_2] - k_2[NO][O_3]$. The importance of organic species in the atmosphere arises because they are readily converted to reactive species (notably peroxy radicals, RO_2), which bring about this conversion of NO to NO_2.

$$RO_2 + NO \rightarrow NO_2 + RO \qquad \text{Equation 9}$$

The initial step in the conversion of VOCs usually involves cleavage of the organic molecule to produce a free radical. This may occur as a result of photolysis, or following attack by OH, O, or O_3:

$$VOC + h\nu, OH, O, O_3 \rightarrow R \quad . \qquad \text{Equation 10}$$

Rapid reaction of the free radical then takes place, often involving oxygen molecules and producing peroxy radicals.

$$R + O_2 \rightarrow RO_2 \qquad \text{Equation 11}$$

Other reactions lead to the formation of hydroxyl (OH) and hydroperoxy (HO_2) radicals.

The importance of organic species in ozone production is underscored by combining the reactions shown in equation 4, 5, 9, and 11.

$$NO_2 + h\nu \rightarrow NO + O \qquad \text{Equation 12}$$

$$O + O_2 \rightarrow O_3 \qquad \text{Equation 13}$$

$$RO_2 + NO \rightarrow NO_2 + RO \qquad \text{Equation 14}$$

$$R + O_2 \rightarrow RO_2 \qquad \text{Equation 15}$$

$$\overline{R + 2O_2 + h\nu \rightarrow RO + O_3}$$

This combination of equations indicates that the net effect of the free radical (plus light) is to bring about the conversion of oxygen to ozone. Note in particular that the oxides of nitrogen are not

consumed in this process, which can thus continue as long as hydrocarbons are present. However, a certain amount of NO_x is required before the process can begin.

The free radicals described above are also involved in the formation of acidic species in the atmosphere. Important reactions include the reaction between OH and SO_2, which ultimately produces sulphuric acid:

$$OH + SO_2 \rightarrow HSO_3 \rightarrow H_2SO_4 \quad . \qquad \text{Equation 16}$$

(The details of the subsequent reactions are still not completely understood, but are known to involve water vapour molecules: Calvert 1981; Moller 1980; Stockwell and Calvert 1983). Production of nitric acid involves a similar reaction between OH and NO_2:

$$OH + NO_2 \rightarrow HNO_3 \quad . \qquad \text{Equation 17}$$

Free radical species and their reaction products are also believed to be involved in the aqueous phase (i.e., in-cloud and in-rain) processes leading to acid production (Chameides and Davis 1982).

Of concern in polluted areas is the formation of peroxyacetyl nitrate (PAN), which is a potent lachrymator. This too is formed as a result of free radical reactions (Demerjian et al. 1974).

All organic compounds are not equally effective in producing the reactive species important in the reactions discussed above. Ideally, each compound should be considered separately, but this approach is not feasible, since upwards of 400 organic species have been identified in the atmosphere (Graedel 1978). It is, therefore, general practice to group organic species into classes, within each of which the reactivities are approximately equal. There is wide variation of the number of classes that may be considered, ranging from four classes for many models (e.g., Demerjian and Schere 1979; Penner 1984) to ten for a large model currently under development for the Province of Ontario (ERT 1984), and as many of thirty-five in one example (Derwent and Hov 1980). An alternative scheme considers the reactivity of individual bonds within the molecules (Killus and Whitten 1982). It should be stressed that this is a very

brief review of the relevant chemistry, omitting a number of the finer details (e.g., the fate of the various reaction products). However, it is clear that any model that is applied to describe the air quality of Edmonton and Calgary will be required to address the details of chemical transformation of all pollutants.

The translation of a chemical mechanism into mathematical terms for inclusion in a model is achieved by first writing down a rate expression for each reaction in the mechanism. For an elementary (i.e., single step) reaction

$$A + B \rightarrow C + D \quad , \qquad \text{Equation 18}$$

the rate expression will be

$$-\frac{d[A]}{dt} = -\frac{d[B]}{dt} = \frac{d[C]}{dt} = \frac{d[D]}{dt} = k\,[A][B] \quad , \qquad \text{Equation 19}$$

where the square brackets denote concentration, and the rate constant, k, is determined experimentally as a function of temperature.

For more complex reactions, i.e., those which, as written, summarize two or more steps, more complex expressions may be found. These, too, must be determined experimentally.

From the complete set of rate expressions those terms relating to an individual chemical species are collected together to form the rate equation for that species. This equation then forms a part of the source/sink term, S, in the general transport equation.

It should be noted that, although atmospheric chemistry represents only a part of one term in the transport equation, it is fundamental to urban air quality modelling for two reasons. First, without atmospheric chemistry there would be essentially no pollution problem, since secondary pollutants such as ozone, PAN, and acids would not be formed.

Second, the nature of the terms contributed by the chemistry is computationally demanding. It is commonly found that 80 percent or more of the computer time is taken up in treating the chemistry. Some details of numerical methods used specifically for solving the chemical part of the equation are discussed in the next section.

2.3 NUMERICAL SOLUTION ALGORITHM

The highly non-linear and coupled form of the governing differential equations in their three-dimensional, temporal form does not allow for a closed form, analytic solution. A solution can only be obtained, and the three-dimensional, temporal form of the equations preserved, if a numerical scheme is employed. The type of numerical schemes considered in this report are applicable to Eulerian models. In Eulerian models, the airshed is divided into a set of grid cells of fixed dimensions, and each of the terms in the differential equation is approximated in terms of finite differences. The purpose of the numerical solution method is to introduce approximations on the spatial and temporal variation of the field variables at a local level (subdomains), such that the partial differential equation can be replaced by a set of algebraic equations. Solution of the algebraic equations gives an approximate solution for the domain of interest.

Further, since the time scales of importance to the chemistry terms are very different from those of the other processes, it is common to use operator splitting in the solution process. That is, it is assumed that the operations of transport and diffusion and chemistry and deposition can be handled separately, with the overall transport equation being solved by the process

$$L_t \, L_c \, C_i \ ,$$

where L_t and L_c represent the operations of transport and diffusion and chemistry and deposition respectively. Economies may be achieved by the following modified grouping:

$$L_t(\Delta t) . \, L_c(2\Delta t) . \, L_t(\Delta t) . \, C_i \ ,$$

which indicates that in advancing the solution by $2\Delta t$, the chemistry is integrated over the full time step after (and before) two half time step advances of the transport and diffusion. A more detailed discussion of this process is given by McRae et al. (1982a).

It should be noted that the final numerical solution, regardless of the type of numerical scheme, is approximate, at least in practical terms. A discretized equation is an algebraic relation connecting the values of a field variable ϕ for a group of grid

points. That only a few grid points participate in a given discretization equation is a consequence of the fragmented nature of the profiles chosen. The value of ϕ at a grid point therefore influences the distribution of ϕ only in its immediate neighbourhood. As the number of grid points becomes very large, the solution of the discretization equations is expected to approach the exact solution of the corresponding differential equation. This follows from the consideration that, as the grid points get closer together, the change in ϕ between neighbouring grid points becomes small, and then the actual details of the profile assumption become unimportant. With this understanding, the error in the numerical solution, defined as the difference between the solution obtained by an analytical method and the numerical method, is a function of the number of discrete grid points used, and depends on how well the local profile assumptions approximate the true variation of the variable.

Different types of numerical schemes arise because of the differences in the assumptions made in expressing the variation of the field variables between grid points and in the derivation of the schemes. A limitation that is common to each scheme will be the error due to use of only a finite number of grid points. Because of the three dimensionality of an urban airshed, elimination of this error would require more grid points than is computationally practical to use. Attention therefore must focus on the physical basis of the scheme.

A large amount of the numerical error can be eliminated by choosing a numerical scheme that accurately expresses the same physical trends as the actual phenomena being modelled (Raithby 1976a,b). An order of magnitude analysis of the terms in the conservation of mass equation using values typical to the planetary boundary layer shows an urban air quality simulation to be a transient, convection-dominated problem with strong sources and cross wind diffusion. This physical understanding can be used in evaluating the different numerical schemes.

Another feature required of the numerical scheme is that it be conservative. A conservative scheme is one that guarantees the conservation of mass at both the local (grid cell) and global level, and not just in the limit as the number of grid points become very large (Patankar 1980). Having a conservative scheme does not necessarily guarantee a more accurate solution, but it is an attribute that lends itself to direct physical interpretation and it provides a basis on which the validity of the model can be assessed.

Whether the scheme is explicit or implicit can also be used in evaluation as this will have a significant effect on the computational efficiency of the method. Explicit methods are subject to very restrictive time steps in order to remain numerically stable and are therefore more costly computationally than implicit formulations.

A great deal of research has been conducted on the performance of different numerical schemes with respect to the above criteria. In the next section the evaluation of the numerical schemes used in the chosen models will be based upon their physical basis and known behaviour under the physical conditions typical of an urban environment.

As was discussed earlier in this section, it is usual to separate the integration of the chemical terms from that of the remainder of transport equation. This is necessary because the time steps involved in the chemistry can be extremely short (fractions of a second). Further, the sets of equations describing the chemistry are generally stiff, in that the time constants for the different species cover a very large range. In practice this means that conventional solution techniques require very short time steps to follow accurately the concentrations of the highly reactive species, yet require a very large number of steps to track the concentrations of the more slowly reacting species. The result is that at best the solution is only achieved at unacceptable cost in computer time, and at worst may be obscured entirely by the accumulation of roundoff and other errors.

Several special techniques are now available for solving stiff sets of equations, including:

1. the algorithm developed by Gear (1971),
2. the asymptotic solution technique, and
3. application of stationary state assumptions.

The asymptotic techniques are claimed to be considerably faster than the Gear algorithm for most problems (Young and Boris 1977), while being capable of achieving an accuracy better than that of the transport calculation (i.e., of the order of one percent).

Stationary state techniques achieve economies by assuming that the most reactive species rapidly achieve a stationary state characterized by a small, steady concentration. The time derivative of the concentration can then be set equal to zero, and the concentration(s) determined by solving the resulting equations. This technique allows a reduction in the number of species for which integration is required, but the major economies arise because the species thus removed are those with the smallest time constants. The stiffness of the problem is thus substantially reduced. However, there is a very real danger that spurious results will be obtained if the stationary state is incorrectly applied, that is, when the time derivative of the concentration of the species in question is actually significantly different from zero. Such assumptions should therefore be used with caution.

3. MODEL IDENTIFICATION, SCREENING AND EVALUATION

3.1 MODEL IDENTIFICATION

Model identification made use of on-line literature search, supplemented by limited manual search (confined to Atmospheric Environment, Environmental Science and Technology and the Journal of the Air Pollution Control Association) and personal knowledge gained in the course of previous reviews of urban air quality models (e.g., CSC 1984). The models identified in this way are listed in Table 3.

All of these models were retrieved in the course of the on-line search. The other two methods of identification therefore confirmed that good coverage of available models was achieved.

A model not identified in the initial search was Hage and Hops, 1982a,b. The model was brought to the attention of the authors during the review of the final report, and it was not possible to perform a detailed model analysis.

3.2 MODEL SCREENING

It was clearly impossible to carry out a detailed evaluation of all models listed in Table 3 to select the most appropriate one for application in Alberta. A screening process was therefore used to produce a short list of models for detailed evaluation.

To ensure that the needs and requirements of future model users are met, the screening criteria were based in part on the responses to a questionnaire submitted to potential users. These responses are summarized in Table 4, and the screening criteria are listed in Table 5. Note that the inclusion of a detailed photochemical mechanism is a necessary screening criterion if secondary pollutants, such as ozone and PAN, are to be treated. However, the screening criteria do not include the need for incorporation of the reactions of SO_2 into the mechanism, even though wet and dry deposition of sulphate is of interest to future users. Sulphur dioxide is very seldom included in urban scale models, so its inclusion as a screening criterion would have proved very restrictive. Instead, a discussion of how SO_2 chemistry can be incorporated is given in Section 3.3.5.

In the course of model screening duplication of models was also eliminated. For example, the model SMOG, currently in the

Table 3 Models Identified

Name	Reference
Takeuchi and Kimura	Takeuchi and Kimura (1977)
Yashikawa and Akiyama	Yashikawa and Akiyama (1977)
URBMET	Bornstein et al. (1985)
GRID	van Egmand and Kesseboam (1983)
van Dop and de Haan	van Dop and de Haan (1983)
Kamst and Lyons	Kamst and Lyons (1982)
Liu and Goodin	Liu and Goodin (1976)
UBL	Ivanyi and Merish (1982)
Melli and Fronza	Melli and Fronza (1982)
Shir and Shieh	Shir and Shieh (1979)
Demuth et al.	Demuth et al. (1982)
McNider	McNider and Pielke (1980)
Egan and Mahoney	Egan and Mahoney (1972)
Bankoff and Hanzerach	Bankoff and Hanzerach (1975)
LIRAQ	McCracken et al. (1978)
IMPACT	Fabrick et al. (1977)
UAM	Reynolds et al. (1973)
McRae et al.	McRae et al. (1982a)
Lagrangian Models	
Lamb and Niemberger	Lamb and Niemberger (1971)
Sklarew	Sklarew et al. (1971)
ADPIL	Knox (1974)
Eschenroeder	Eschenroeder et al. (1972)
ARMAX (Stochastic)	Finzi and Tebaldi (1982)
CDM (Statistical)	Irwin and Brown (1985)
Bingfelt et al. (Gaussian)	Bingfelt et al. (1974)
Husain et al. (Gaussian)	Husain et al. (1981)
CRSTER (Gaussian)	US EPA (1977)
Nieuwstadt (Gaussian)	Goumans, H.H.J.M. and Clarenburg, L.A. (1977)
PARIS (Plume)	Seigneur et al. (1983)
Brewer et al. (Box)	Brewer et al. (1981)
ASP (Box)	Long et al. (1984)
ATDL (Box)	Hanna (1978)
MGM (Gaussian)	Ritchie et al. (1983)
Long et al. (Box)	Long et al. (1983)
Laird et al. (Box)	Laird et al. (1982)
AQDM (Gaussian)	TRW (1969)
RAM (Gaussian)	Turner and Novak (1978)
Other	
PAL (Gaussian)	Petersen (1978)
Leahey (Box)	Leahey (1975)
McCracken et al. (Box)	McCracken et al. (1977)

Table 4. Summary of questionnaire responses.

Question	Response
Probable model applications	1. Impact assessment: a) new and existing sources b) air quality downwind of cities c) transportation and land use planning 2. Data analysis a) control strategy development b) trends and forecasts c) separation of meteorological and source influences d) source identification 3. Research a) extent of photochemical pollution b) additional species to be monitored c) need for VOC emission inventory 4. Episodes a) diagnosis b) real-time control
Will applications be similar for all urban centres	Yes
Important pollutants (rank order)	Oxidants, ozone, oxides of nitrogen, particulate matter, carbon monoxide, dry and wet sulphate deposition, dry and wet nitrate deposition, sulphur dioxide
Spatial scales of interest (rank order)	Urban, regional, local
Important time scales (rank order)	Hourly, daily, seasonal, annual
Special meteorological and other conditions which may be encountered	ARCTIC air mass inversion pre-chinook (Calgary) quasistationary fronts "Indian summer" - fall stagnation topography (Calgary) river valley (Edmonton)
Other considerations	Model credibility is of the utmost importance. Eulerian model required

Table 5 Screening Criteria

Eulerian framework	-	three dimensional wind and concentration fields
Detailed photochemical mechanism	-	
Detailed model descriptions available	-	model documentation
	-	test cases available
	-	sensitivity and validation tests

possession of Alberta Environment, is essentially identical to IMPACT, and was therefore not considered separately.

The screening process resulted in the retention of four models, which were carried forward for detailed evaluation. These models are listed in Table 6, and are described in Section 3.3.

3.3 DESCRIPTION OF MODELS

As described in Section 2, the basis for each of the models considered in this report is the conservation of mass equation, where due consideration has been given to the averaging of the fundamental equation as required for use in a numerical model with finite space and time increments. With the use of K theory to model the turbulent correlations, the governing differential equation for a particular pollutant species is:

$$\frac{\partial C_i}{\partial t} + \frac{\partial}{\partial x} uC_i + \frac{\partial}{\partial y} vC_i + \frac{\partial}{\partial z} wC_i = \frac{\partial}{\partial x} K_H \frac{\partial C_i}{\partial x} + \frac{\partial}{\partial y} K_H \frac{\partial C_i}{\partial y} + \frac{\partial}{\partial z} K_V \frac{\partial C_i}{\partial z} + S_i$$

Equation 20

where K_H and K_V are the horizontal and vertical diffusion coefficients respectively.

In this form the equation expresses the horizontal and vertical variation of wind and concentration. It is also in a form applicable to a Cartesian co-ordinate system. This form of the equation will be used as the standard by which the formulations of the models will be compared.

The models are all similar in that they are Eulerian, use prescribed diffusivity profiles, and decouple the wind field from the mass conservation equation. How each model handles these features, and their treatment of the reactive chemistry and source emissions, is unique. In this section, brief descriptions of each of the models will be presented with attention focusing on the major manipulations made to the governing differential equation and on the most significant advantages and limitations. The more specific details of the models will be presented in the Section 3.4 (model evaluation).

Table 6. Models surviving screening.

Name	Reference
LIRAQ	McCracken et al. (1978)
Urban Airshed Model (UAM)	Reynolds et al. (1973)
McRae et al.	McCrae et al. (1982)
IMPACT	Fabrick et al. (1977)

3.3.1 LIRAQ

The LIRAQ model (McCracken et al. 1977) was originally developed in 1977 at the Lawrence Livermore Laboratory of the University of California for use in the San Francisco Bay area. The LIRAQ model is different from the other models in that it uses a simplified Eulerian formulation of the continuity equation. This includes a complete treatment of the two horizontal dimensions and a vertically averaged treatment in the vertical dimension.

The rationale for this approach concerns the role of the temperature inversion in determining air quality. It was argued by McCracken et al. (1978) that an atmospheric temperature inversion is almost always present during periods of poor air quality. The inversion effectively constrains the vertical mixing of surface pollutant emissions. Because the vertical structure of the atmosphere is often poorly known and difficult or expensive to observe, the atmosphere below the inversion is treated as a single layer. This formulation will reduce the amount of input data and computer time needed by the model.

This vertical averaging requires that the governing equation be integrated in the vertical from a lower reference level $Z\phi$ to the top of the mixed layer $H(x,y,t)$. To perform this integration a vertical functional dependence of the concentration and horizontal wind is assumed. The wind components are written in the following manner:

$$u(x,y,z,t) = U_m\ (x,y,t) \cdot \left(\frac{Z}{Z_m}\right)^n \qquad \text{Equation 21a}$$

$$v(x,y,z,t) = V_m\ (x,y,t) \cdot \left(\frac{Z}{Z_m}\right)^n \qquad \text{Equation 21b}$$

where U_m and V_m are the velocity components at reference height Z_m, and n is a stability dependent parameter (approximately $^1/_7$).

The concentration profile is represented by

$$C_i\ (x,y,z,t) = a_i\ (x,y,t) + b_i\ (x,y,t) \cdot \ln\ (\frac{Z}{Z\phi}) \quad , \qquad \text{Equation 22}$$

where a_i and b_i are parameters dependent on the mixing depth, source strength, deposition velocity, and the diffusivity at the height $Z\phi$. Below $Z\phi$ the concentration is assumed constant with height.

Substitution of equations 21a and 21b and 22 into 20 and integration between $Z\phi$ and H yields the governing differential equation for LIRAQ:

$$\frac{\partial}{\partial t}\ (\Delta H \cdot \bar{C}i) + \frac{\partial}{\partial x}\ (U \cdot \Delta H \cdot \bar{C}i) + \frac{\partial}{\partial y}\ (V \cdot \Delta H \cdot \bar{C}i) + Wi =$$

$$\frac{\partial}{\partial x}\ (K_H \frac{\partial}{\partial x}\ [\Delta H \cdot \bar{C}i]) + \frac{\partial}{\partial y}\ (K_H \frac{\partial}{\partial y}\ [\Delta H \cdot \bar{C}i]) + \bar{S}i \cdot \Delta H \quad , \qquad \text{Equation 23}$$

where $\bar{C}i$ is the vertically averaged concentration of pollutant, $\bar{S}i$ is the vertically averaged source term, and ΔH is the difference between H and $Z\phi$. The term Wi represents the net effective flux of pollutant transported through the top of the solution domain, and is given by:

$$Wi = \begin{cases} W_H \cdot \bar{C}(x,y,H,t) & W_H > 0 \\ 0 & W_H = 0 \\ W_H \cdot Ct & W_H < 0 \quad , \end{cases} \qquad \text{Equation 24}$$

where W_H is the velocity at the top of the region and Ct is the boundary concentration at H. Specifying fluxes at the top simulates the different processes associated with a transient inversion height.

Concentrations predicted by LIRAQ are vertically averaged values, though application of Equation 22 does enable one to obtain an estimate of the ground level values. The parameters a_i and b_i are derived from a balance between diffusion, deposition, and pollu-

tant emissions at the surface. If the source flux is larger than deposition, then the near ground level concentration will be higher than the vertical average concentration and vice versa.

The major limitation of LIRAQ is that it does not have a layer of grid cells above the inversion height. This restriction does not allow LIRAQ to handle the entrainment into the mixed layer of pollutants that enter the inversion either from elevated point source emissions or at the time the stable layer forms during the night. Current work on LIRAQ includes the addition of an elevated layer (Penner 1984).

LIRAQ incorporates a 59 reaction mechanism of 29 chemical species (Penner and Walton 1982). It is based on the mechanism described by Hecht et al. (1974), but incorporates more recent rate constant data, and the reactions of aromatic hydrocarbons have been added. The mechanism has been validated against smog chamber data, but reactions of SO_2 are not included.

This mechanism is interesting in that it accounts for "lumping" of organic compounds by incorporating reactivity weighting of emissions, rather than weighting of rate constants as is done in other mechanisms. The advantage of this approach is that shifts in the composition of organic emission are automatically accommodated. However, there are also potential problems, as noted by Leone and Seinfeld (1984), who have recommended that the approach be subjected to detailed re-evaluation.

3.3.2 Urban Airshed Model and McRae et al.

The general descriptions of the Urban Airshed Model (Reynolds et al. 1973) and the model of McRae, Goodin, and Seinfeld (McRae et al. 1982a) can be presented together because of the similarity in their general formulation. Differences exist in their handling of the model components and parametrizations. The model of McRae et al., being developed more recently, possesses the state-of-the-art parametrizations. These differences are documented in Section 3.4.

The Urban Airshed Model (UAM) was originally developed in 1973 by Systems Applications Inc. in California. The model of McRae et al. is basically the final product of the doctoral work of Gregory McRae. This was completed in 1981.

A unique attribute of these models is that to facilitate the application of finite difference methods, the vertical dimension is normalized to the distance between the bottom and top of the modelling region. This is accomplished by defining a new independent variable:

$$\rho = \frac{Z - h(x,y)}{H(x,y,t) - h(x,y)} \quad , \qquad \text{Equation 25}$$

where $h(x,y)$ is the terrain height, and $H(x,y,t)$ is the time-dependent elevation of the top of the region.

This transformation eliminates irregularities in the solution domain due to the irregular base and the irregular and transient top of the solution domain. By transforming the solution domain into a region, fixed in vertical extent between the limits of $\rho = 0$ and $\rho = 1$, the equation is much more amenable to numerical solution. Also, the transformation ensures that the normal at the lower boundary is always parallel to the vertical axis, which makes boundary conditions much easier to implement.

Upon performing this change of variable and after simplification (see McRae et al. 1982a), the following equation results.

$$\frac{\partial}{\partial t}(\Delta H \cdot Ci) + \frac{\partial}{\partial x}(U \cdot \Delta H \cdot Ci) + \frac{\partial}{\partial x}(V \cdot \Delta H \cdot Ci) + \frac{\partial}{\partial \rho}(W \cdot Ci) =$$

$$\frac{\partial}{\partial x}(K_H \cdot \Delta H \cdot \frac{\partial Ci}{\partial x}) + \frac{\partial}{\partial x}(K_H \cdot \Delta H \cdot \frac{\partial Ci}{\partial x}) + \frac{\partial}{\partial \rho}(\frac{Kv}{\Delta H}\frac{\partial Ci}{\partial \rho}) + Si\Delta H \quad ,$$

where

$$W = w - u(\frac{\partial h}{\partial x} + \rho\frac{\partial \Delta H}{\partial x}) - v(\frac{\partial h}{\partial y} + \rho\frac{\partial \Delta H}{\partial y}) - \rho\frac{\partial \Delta H}{\partial t}$$

$$\Delta H = H - h \qquad \text{Equation 26}$$

The terms in W are all known, being provided by the terrain $(\frac{\partial h}{\partial x}, \frac{\partial h}{\partial y})$, knowledge of the specified variation of the top of the

solution domain ($\frac{\partial \Delta H}{\partial x}$, $\frac{\partial \Delta H}{\partial y}$, $\frac{\partial \Delta H}{\partial t}$), or the wind field specification (u, v, w). With the specification of boundary and initial conditions, solution of Equation 26 yields the predictions obtained by the Urban Airshed and McRae models.

It is to be noted that the models allow cells to be specified in the vertical. These cells may include all or part of the mixed layer or can extend into an elevated inversion layer if one exists. No a priori assumptions concerning the vertical profile of the winds or pollutant concentrations are made. The vertical resolution depends on the number of vertical layers used. Ground level concentrations are taken to be the concentrations computed in the lowest level of cells.

A model formulation that combines time-varying grid spacing and vertically varying diffusivity profiles allows considerable flexibility in the type of scenarios that can be modelled. For example, calculations can be performed in the mixed layer only by specifying the top of the solution domain to coincide with the base of the inversion. To facilitate the calculation of pollutant concentrations within the inversion, grid cells can be added which are bounded by the base and top of the inversion. It also allows scenarios such as one in which ozone or other pollutants trapped aloft at night and fumigated the next day.

In contrast to the similarity of their treatment of transport and diffusion, the two models use very different chemical mechanisms.

The Urban Airshed Model uses the Carbon Bond Mechanism (CBM), which was developed by Systems Applications Incorporated of California (Whitten and Hogo 1977), and has subsequently undergone major updates. The current version is known as CBMX, Whitten et al. 1985; the previous versions were CBMI, CBMII and CBMII.

The CBM is unique in the approach adopted to the grouping of organic compounds, in that molecules of similar types (e.g., aldehydes or olefins) are not grouped together as in as do many other mechanisms. Rather, each molecule is considered to be made up of

building blocks, each of which has its own reactivity. The specific building blocks considered in CBM III are the olefinic double bond, the aromatic moiety, the carbonyl group, the paraffinic carbon atom, and benzaldehyde. Ethylene is also segregated as a separate species.

This concept of individual groups within a molecule retaining, approximately, their unique properties is well established in chemistry. It has been used, for example, by Benson (1968) in the estimation of thermochemical properties, and is widely invoked in the determination of molecular structure from infrared spectra.

In its present form, CBM X includes 146 reactions of 65 species, but does not include reactions of SO_2. However, three reactions for the conversion of SO_2 to sulphate were however added to CBM in a modelling study carried out by Meagher and Luria (1982).

The CBM has been validated against smog chamber data from the Statewide Air Pollution Research Centre (SAPRC) at the University of California at Riverside, and from the University of North Carolina. It has also been included in other computer models, notably the Regional Transport Model and the Reactive Plume Model. It is also intended that a version of CBM III be incorporated in the US EPA's Regional Oxidant Model (Lamb 1983). It should be noted that the version of UAM released by the US EPA contains CBM II, which is not the most recent version.

McRae et al. (1982a) have included in their model an updated version of the mechanism by Falls and Seinfeld (1978). (This, in turn, was a refinement of the Hecht et al. (1974) mechanism, upon which the LIRAQ chemistry is based). It now includes 52 reactions of 31 chemical species, including five lumped organic classes (higher olefins, paraffins, formaldehyde, other aldehydes and aromatics). Ethylene is also treated separately. The mechanism was validated against SAPRC smog chamber data, but does not include the reactions of SO_2.

Examples of the use of this mechanism in models of various types are given by Brewer and Remsberg (1980), Bazzell and Peters (1981), Wakelyn and Gregory (1980), McRae and Seinfeld (1983) and

Balko and Peters (1983). In the latter case, reactions of SO_2 were added.

Reviews by Dunker et al. (1984) and Jeffries et al. (1981) point out that this mechanism does not treat aldehyde photolysis correctly. In view of the good agreement with smog chamber data, this indicates that the mechanism probably contains a further compensating error or errors. A detailed analysis by Leone and Seinfeld (1984) has identified the aromatic chemistry as requiring updating.

3.3.3 IMPACT

The IMPACT urban air quality model (Fabrick et al. 1977) was developed by Science Applications Inc. in 1977. The model, in principle, is the same as the Urban Airshed and McRae models in terms of being able to treat multiple layers, multiple sources, effects of terrain, and chemical reactions. It therefore has many of the same attributes described in the preceding section. These will not be repeated here.

Differences, as before, exist in its treatment of the model parametrizations, and also in the fact that it does not use a vertical co-ordinate transformation. The IMPACT model retains the original Cartesian formulation as in Equation 20.

Opting not to transform the vertical dimension puts the model at a slight disadvantage in relation to UAM and McRae et al. First, because the grid cells must remain rectangular, the true topography can only be represented within the resolution dictated by the choice of the grid dimensions ΔX, ΔY, and ΔZ. This is shown in Figure 1. This requires cruder approximations of how the terrain will deflect wind flow than do the other models. The co-ordinate system used by UAM and McRae accounts for variable terrain gradients. Also, the IMPACT formulation does not allow the top of the solution domain to vary with time without using very complex numerical interpolation schemes. With a simple Cartesian grid, if the top of the solution domain were to vary with time, a different grid would result at each time step. A transient solution would then require a temporal and a spatial interpolation routine to relate the computed

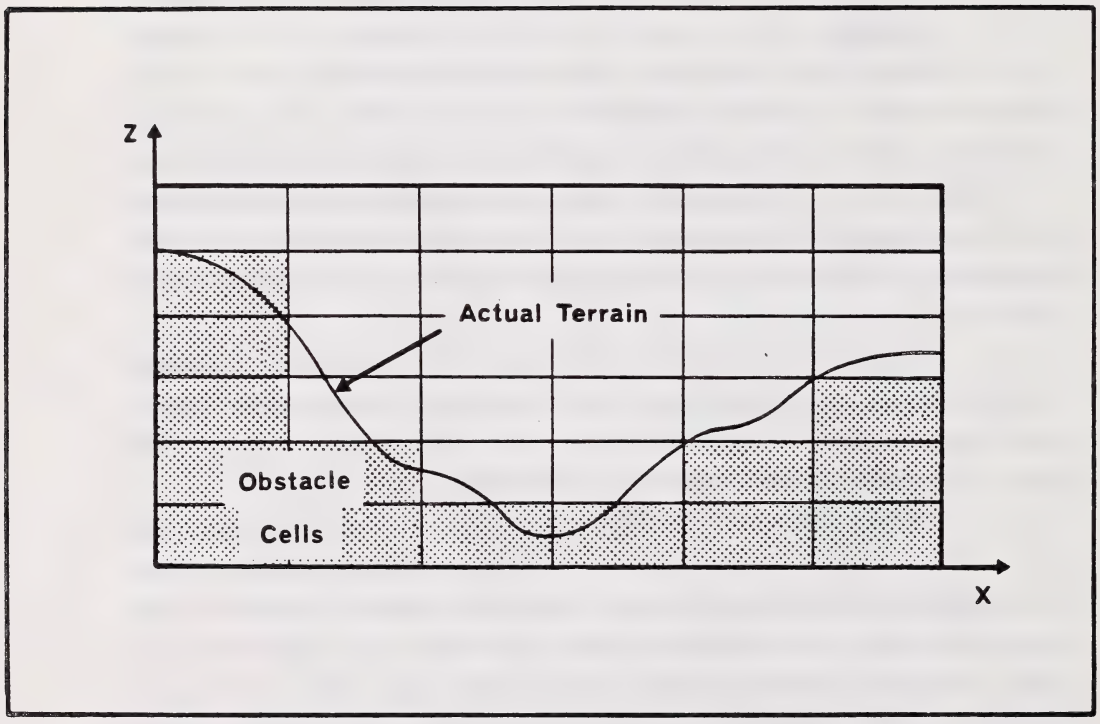

Figure 1. Two-dimensional representation of terrain in IMPACT.

variables from the grid at time t_1 to those at t_2. The current form of IMPACT does not have an interpolation routine to handle this problem.

This restriction limits to some extent the range of applicability of the model. For example, it could not be used effectively to model urban air quality during the growth of the mixed layer if all of the grid cells were put in the boundary layer. In this instance, it would have to be assumed that the mixed layer height remains fixed in time, or some grid cells would have to be put above the inversion, which would leave a coarser resolution in the mixed layer. In general, the IMPACT model must rely more heavily on empirical relations or diagnostic formulae in order to predict the effects of temporal variation of the mixing height.

IMPACT offers at least three options as far as the chemical mechanism is concerned. The most sophisticated of these is essentially identical with the mechanism described by Hecht et al. (1974), which considers the reactions of three organic classes as typified by propylene, butane, and a mixture of formaldehyde and acetaldehyde.

3.4 EVALUATION

In this section, the different parametrizations and submodules used in each of the models will be discussed and compared. To complement the general descriptions of the previous section, the turbulent diffusion coefficients, elevated sources, dry deposition, wind field generator, and numerical algorithm will be presented. These are the essential features of the models and a detailed comparison of these, together with the chemistry, will provide sufficient information on which to base a final decision.

3.4.1 Turbulent Diffusion Coefficients

As described earlier, each of the models covered in this report adopts K theory to represent the transport of pollutants by the turbulent motion of the atmosphere. The turbulent motion is

three-dimensional and it is therefore necessary to prescribe turbulent diffusivities for each co-ordinate direction.

The relative importance of turbulent diffusion in transporting airborne pollutants in the horizontal and vertical directions is quite different. In the horizontal, the transport is dominated by mean wind advection. This is particularly apparent when a scale analysis is done between horizontal advection and diffusion. Taking the typical mesoscale meteorological values U=5 m/s, ΔX=5 km, and Kx=50 m^2/s, the magnitude of the advection and diffusion terms would be:

$$\frac{\partial}{\partial x} UCi \simeq \frac{UC}{\Delta x} = \frac{5Ci}{5000} = 1(10^{-3})\ Ci \qquad \text{Equation 27}$$

$$\frac{\partial}{\partial x} Kx \frac{\partial Ci}{\partial x} \simeq \frac{KxCi}{\Delta x^2} = \frac{50\ Ci}{(5000)^2} = 2(10)^{-6}\ Ci. \qquad \text{Equation 28}$$

The three orders of magnitude difference indicates the strength of advection relative to diffusion. The value of Kx used in the above analysis is the value used in UAM. Because at the above difference, not as much attention need be given to the development of horizontal diffusivity profiles which take into account all the relevant meteorological and topographic features. Also, to support this assertion further, it has been found that the predicted concentrations are insensitive to the choice of Kx. For example, Liu et al. (1977) studied the effect of changes in Kx (0-500 m^2/s) and concluded that the effect on concentration predictions for area wide averages is less than two percent.

Table 7 summarizes the different horizontal diffusivity profiles that are used. Comparison shows that the model used by LIRAQ embodies more fundamental physics than any of the others. Its initial derivation is based upon the dissipation of turbulent kinetic energy, and the layer averaged form shows that it is determined independently at all points on the grid and that it is spatially and temporally dependent on the wind velocity. This is in contrast to

Table 7. Horizontal diffusivity models.

LIRAQ	$K_H = A \cdot \frac{V_o}{Z_\phi^n} \left[\frac{1}{nH}(H^{3n} - Z_\phi^{3n})\right]^{1/3} \Delta S$ A = constant, V_o = surface velocity ΔS = horizontal grid spacing H = inversion height n = exponent (Eq'n. 21)
IMPACT	$K_H = \alpha \cdot K_v$ α = stability dependent factor
UAM	$K_H = 50\ m^2/s$
McRae	$K_H = 0.1.W_* H$ W_* = scaling velocity H = inversion height

the simplicity of the other formulations that are, at most, dependent on atmospheric stability and height.

It should be stressed that horizontal diffusion is not a dominant process and therefore the specification of a complex horizontal diffusivity is not critical. This contention is further supported when consideration is given to the fact that the physical horizontal diffusion can be partly contaminated with numerical diffusion. Unless special care is taken, numerical diffusion can exceed the physical diffusion. This applies particularly to the LIRAQ model. In the version that handles reactive chemistry, simple upwind differencing is used on the advective term. This form of differencing can introduce significant amounts of false diffusion in certain flow situations. The false diffusion coefficient for straight upwinding can be estimated by

$$Km_f = \frac{\vec{V} \cdot \Delta x \cdot \Delta y \cdot \mathrm{Sin}\,(2\theta)}{4(\Delta y\,\mathrm{Sin}^3\theta + \Delta x\,\mathrm{Cos}^3\theta)} \qquad \text{Equation 29}$$

(see DeVahl Davis, and Mallinson 1972). In the worst case θ, the angle between the velocity vector and the grid lines will be 45°. Taking $\Delta x = \Delta y$, this reduces to

$$Km_f = 0.707 \cdot \Delta x \cdot \vec{V} \quad . \qquad \text{Equation 30}$$

For typical values of Δx and $\vec{V}$ (1000 m, 5 m s^{-1}), the false diffusion coefficient is 3500 m^2 s^{-1}. Using these same values with an inversion height of 1000 m, the LIRAQ model will give a value of Km = 65 m^2 s^{-1}. In this worst case, the effects of false diffusion invalidate the careful treatment given to the formulation of the physical diffusion coefficient.

In direct contrast to horizontal diffusion, in the vertical direction turbulent diffusion is the dominant process in transporting pollutants. Therefore, at the outset, it should be remarked that a variety of different formulations exist. These formulations attempt to characterize the vertical turbulent diffusivity in terms of atmospheric stability, surface characteristics and conditions, and wind and temperature variations through the boundary layer. A particular complication in the selection of the more complex forms is the lack of suitably detailed measurements of the necessary atmospheric para-

meters. A guiding principle in evaluating different models is to note which ones employ those parameters that are readily available or can be easily estimated.

Summarized in Table 8 are the various formulations used for the vertical diffusivity. In all cases, except LIRAQ, the diffusivities vary with both height and stability. In LIRAQ, because it is vertically averaged, there is only a need to have a diffusivity at the surface. The formulation used by LIRAQ is a direct analogy with the eddy viscosity used for momentum. At the layer top, the other place where turbulent diffusion can occur, it is assumed in LIRAQ that the material exchange between the mixed layer and the inversion layer resulting from turbulent transport can be included in the net advective flux term Equation 24.

The diffusivity profile used by IMPACT is strictly a function of wind speed and stability. A plot of this profile is shown in Figure 2 for an unstable mixed layer capped by a strong inversion with neutrally stable air above. Also shown is the profile predicted by the McRae model. The most significant difference between the two is that the McRae profile is a smooth, continuous function that scales with the inversion height. Above the inversion, the diffusivity is held fixed at a very small value. The difference in Kv above the inversion is significant between the models and could change the predicted air quality impact of plumes that penetrate the inversion.

A version of IMPACT has the option of using the Myrup/Ranzieri vertical diffusivity formulation. This formulation has the same shape as the McRae model shown in Figure 2. The Myrup/Ranzieri profile would enhance the ability of IMPACT to predict vertical diffusion.

The profiles used in the UAM, while not shown on Figure 2, are quite similar to the diffusivity profile of McRae. The formula presented in Table 8, which was taken from the original paper (Reynolds et al. 1973), expresses the variation of Kv with height through the assumed form of the distribution and with space and time through the horizontal wind components. This form has been updated to include surface roughness, height of the inversion, and the three stability classes.

Table 8. Vertical turbulent diffusivities.

LIRAQ	$Kv_o = 0.1 \cdot k_o \cdot U_1$ k_o = von Karman's constant U_1 = reference velocity
IMPACT	$Kv = k_o \cdot u \cdot \sigma_\varepsilon \cdot \ell$ k_o = von Karman's constant u = wind speed σ_ε = stability-dependent disperion parameter ℓ = stability-dependent turbulent length scale
UAM	$Kv = \begin{cases} (2.5\,\vec{V}-77.3)\,\rho + 30.9 & 0 \leq \rho \leq 0.4 \\ \vec{V} & 0.4 < \rho \leq 0.8 \\ 5(31 - \vec{V})\cdot\rho + 5\vec{V}-124 & 0.3 < \rho \leq 1.0 \end{cases}$ $\vec{V} = 0.85\,(u^2 + v^2)^{1/2} + 232$ ρ = normalized vertical scale

continued ...

Table 8. Concluded.

McRae	Neutral

$$Kv = K_o \cdot u_* \cdot z \cdot \exp\left(-8\,\frac{zf}{u_*}\right)$$

Stable

$$Kv = K(H) + \left(\frac{H-Z}{H-L}\right)^2 \left\{K(L)-K(H) + [Z-L]\left(\frac{2K}{2Z}_{Z=L} + 2\left(\frac{K(L) - K(H)}{H - L}\right)\right)\right\}$$

$$K(L) = 0.025\, k_o\, u_*\, L$$
$$K(H) = 0.05\, K(L)$$
$$H = 0.22\,(u_*) f\,\left(\frac{fL}{u_*}\right)^{1/2}$$

Unstable

$$Z_i 5(k_o \frac{Z}{H})^{4/3}\left[1 - 15\left(\frac{Z}{H}\right)\right]^{1/4} \qquad 0 \leq \frac{Z}{H} < 0.05$$

$$a + b\left(\frac{Z}{H}\right) + C\left(\frac{Z}{H}\right)^2 + d\left(\frac{Z}{H}\right)^3 \qquad 0.05 \leq \frac{Z}{H} \leq 0.6$$

$$\frac{Kv}{w_* H} = aa - \exp\left[6 - 10\left(\frac{Z}{H}\right)\right] \qquad 0.6 < \frac{Z}{H} \leq 1.1$$

$$0.0013 \qquad \frac{Z}{H} > 1.1$$

a, b, c, d, e, aa = constants, k_o = von Karman's constant
u_* = shear velocity, f = coriolis parameter
L = Monin Obukhov length scale
H = inversion height, w_* = convective scale velocity

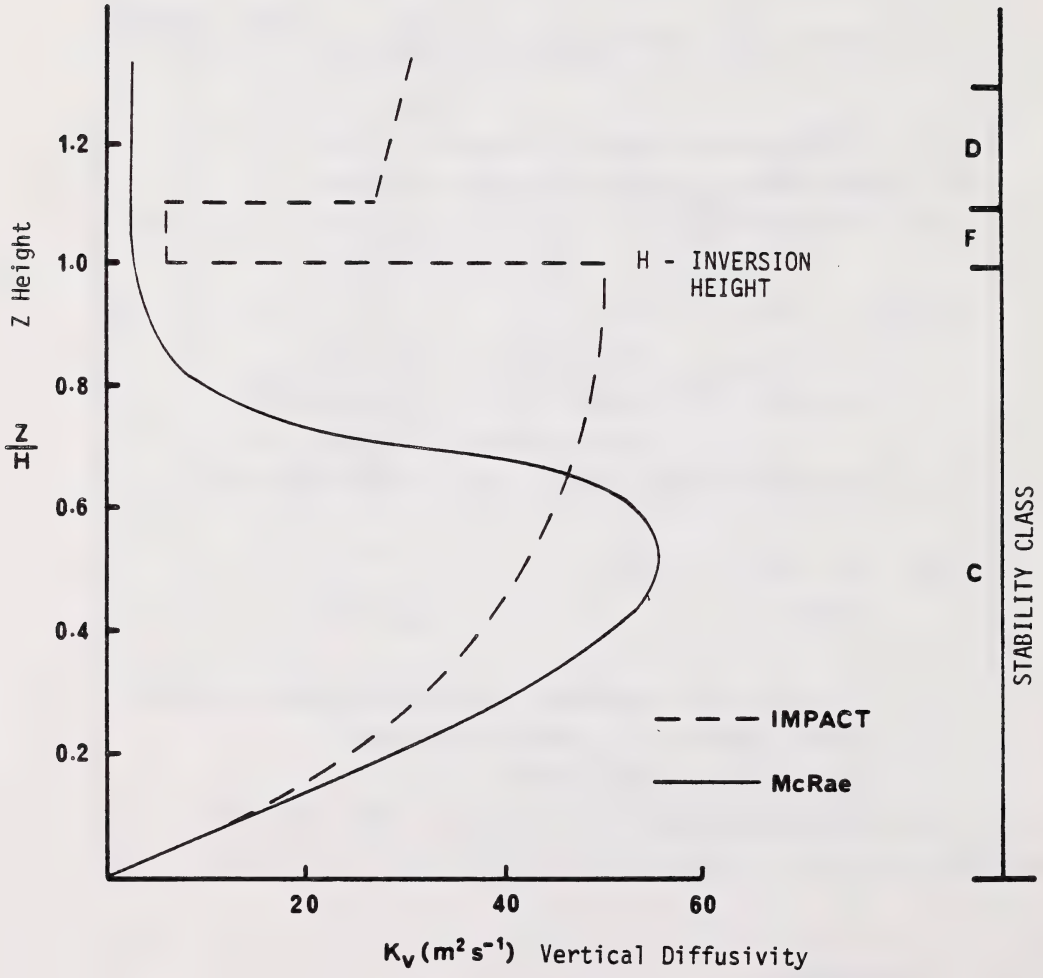

Figure 2. Vertical diffusivity profiles (H - inversion height).

In light of the limited treatment of the inversion layer in LIRAQ, other models would be better suited for applications in which large elevated point sources are important or multiple day simulations are to be performed. The other models allow treatment of such situations as surface based inversions capped by a layer of neutrally stable air or a mixed layer capped by a stable layer. It is felt that the IMPACT profile is at a slight disadvantage as its larger value of Kv above an inversion and in an unstable boundary layer, at the base of the inversion may "overestimate" the turbulent diffusion. The UAM and McRae profiles are by far the most physically sound formulations, having been derived from experimental data and turbulence theory. The profiles, while being complex, are based upon meteorological data that are readily available (surface roughness, surface shear stress and heat flux, inversion height, wind speed).

3.4.2 Elevated Sources (Embedded Plumes)

In this section the treatment of fixed elevated sources (stacks) will be compared. Emissions from mobile sources, distributed area sources (e.g., space heating), and other stationary sources that do not emit pollutants from tall stacks are generally considered to be in the ground-level source category and can be included in the boundary conditions.

The distinction between stationary sources treated as either ground-level or elevated sources is not always clear-cut. For example, industrial plumes, because of their high temperature, are influenced to a large extent by buoyancy. Therefore, due to plume rise, a plume emitted close to the ground will influence the air quality more as an elevated rather than as a ground source. The individual model treatments are presented below, and a summary is found in Table 9.

As discussed in Section 2, it is important that dispersion be accounted for when initially specifying elevated sources. Neglect of this may cause unrealist high concentrations close to the source. Without subgrid scale resolution, the pollutant is assumed to be instantly and uniformly dispersed throughout the grid cell in which it is emitted. This leads to an overestimate of concentration for points outside the plume, and an underestimate for points inside the plume. This situation will persist until the plume cross-section

Table 9. Treatment of elevated sources.

Model	Ground Source Distinction	Plume Rise	Dispersion	Treatment of Inversion Emissions
LIRAQ	h_s < 30 m	-	well mixed	$S_i = \begin{cases} 0 & H < 100 \text{ m} \\ \frac{Q_i}{2H}[1+\sin(\frac{H-125}{50}) \cdot \pi] & 100 < H < 150 \text{ m} \\ \frac{Q_i}{H} & H > 150 \text{ m} \end{cases}$
IMPACT	$h_s < \Delta Z$	Briggs	well mixed into one cell	
UAM	$h_s < \Delta Z_1$ $\Delta Z_1 \approx 50$ m	Briggs	PARIS submodel	
McRae	$h_s = h_p < \Delta Z_1$ h_p = plume rise	Briggs	Gaussian plume dispersing downwind $u \cdot \delta t$, δt averaging time of wind field	Briggs (1975), accounts for penetration into inversion.

approaches the grid cell dimensions. Only in the UAM and McRae models is this effect considered. The UAM uses the PARIS submodel to calculate the effects of dispersion (Seigneur et al. 1983). The PARIS submodel uses Gaussian theory to determine plume spread. If the plume spread is less than the dimensions of the grid cell that it is in, then concentrations are calculated locally. Only when the plume spread exceeds the grid dimensions is it included as a source in the UAM.

Plume rise is calculated by the Brigg's formula. This requires knowledge of the heat flux of the effluents and local meteorological conditions as input. If this is not available then the stack height is used in all calculations.

The McRae model allows the plume to disperse downwind a distance of $U \cdot \delta t$, and in the vertical and lateral directions by Gaussian plume theory. This determines the mass of effluent in each cell. Dividing by the cell volume determines the magnitude of the source contribution.

The treatment of elevated sources used in IMPACT is to assume that all of the stack effluent is injected into a single cell at an elevation given by the sum of the stack height and plume rise.

In all the models, if the effective emission height is above the inversion height, the source is not considered further in the simulation. A feature is incorporated in LIRAQ that varies the percentage of the emissions which stay in the boundary layer for inversion heights between 100 and 150 m. This feature was included to accommodate the specific stack and meteorological conditions of the San Francisco Bay area for which the model was originally developed.

3.4.3 Dry Deposition

The removal of pollutants due to interaction with the ground is a process that can significantly influence concentration levels. It is a difficult problem to include all the relevant physics in the parametrization. As shown in Table 10, all models describe the deposition rate by a single quantity, the deposition

Table 10. Deposition velocity.

LIRAQ, IMPACT	$v_g = v_g(C_i)$ = constant
UAM	$v_g = \alpha \cdot v_g(C_i)$ = constant α = land use factor
McRae	$v_g = \frac{k_o \cdot u_r(1 - \frac{Cd}{Cr})}{(\int_{z_\phi}^{z_r} \Phi_m \frac{dz}{z})[(\frac{Sc}{Pr})^{2/3} + \int_{z_\phi}^{z_r} \Phi_p \frac{dz}{z}]}$ k_o = von Karman's constant r = reference quantity Sc = Schmidt number Pr = Prandtl number Φ_m, Φ_p = stability-dependent functions

velocity Vg. When multiplied by concentration, this gives the flux of material to the ground.

In the simplest cases (LIRAQ, IMPACT), the deposition velocity is specified as a constant dependent on the pollutant species. The UAM takes this one step further by modifying Vg by a factor based on the land type. This introduces a limited amount of spatial variation.

In McRae et al., an upper limit expression was developed for Vg in terms of transport processes and the concentration at a reference point above the surface. The expression shows a significant improvement over the other models as it allows the removal rate to be varied through the ratio Cd/Cr, and also accounts for variation in surface removal due to diurnal changes through the stability-dependent functions Øm and Øp. The unique characteristics of the particular pollutant are introduced through the Schmidt-Prandtl number, which is the ratio of mass to thermal diffusivities.

3.4.4 Wind Field Generation

A key input to urban-scale air pollution models is an accurately specified, mass-consistent wind field. Because it is not practical to solve the full Navier-Stokes equations, simpler objective analysis procedures are used. The most common approach for generating a gridded wind field is first to interpolate surface and upper level data within the airshed to the chosen mesh. Then, with the initial field established, an objective analysis procedure is employed to adjust the wind vectors at each grid point so that appropriate physical constraints are satisfied.

All of the wind field models considered here are similar in their general approach. In each case, mass conservation is used as the physical constraint, and each requires a certain amount of empirical information (specification of constants) to ensure that realistic wind fields are generated. The mathematical formulation of the models is quite different, depending on what features the model incorporates. These mathematical differences will not be presented

here. These can be found in the original papers. Attention will focus on the general features of the models.

The choice of the wind field model is frequently dictated by the nature of the intended application. Since wind data do not usually exist for every part of the region being modelled, judgements must often be made with regard to the way in which wind velocities should be estimated in these areas and whether the calculated velocities are an adequate representation of the expected flow fields. Making such judgements requires experience and knowledge of the meteorology of the area. In light of this, the wind field model used in each model will not have a significant effect on the model selection process. That is, a wind field model should be developed/ selected independently of the urban air quality model, with guidance given by the specific meteorology and topography of the region.

The MASCON model (Dickerson 1978) was developed to prepare wind inputs for the LIRAQ model. Inputs to MASCON are the inversion height, surface wind, and topography of the region. Because of the layer averaging of LIRAQ, MASCON was developed to provide a mass flux field. The mass flux into each grid cell is balanced by the outward flux and changes in the mixing depth so that there is no accumulation or depletion of mass within a cell. Another feature of MASCON is the turning of the wind around topography and channelling of the winds through valleys and mountain passes. The model requires the specification of constant that determines the relative adjustments allowed in the horizontal and vertical fields. The accurate choice of this constant requires an appreciation of the winds in the modelling area.

The impact model uses the WEST wind field model (Sklarew and Wilson 1976). Its mathematical treatment is very similar to MASCON in that a choice is given to the user in the adjustment of horizontal and vertical wind fields. A difference is that it incorporates vertical resolution and also has constants that can be specified to represent different stabilities over the region. Along with requiring inversion heights, surface winds, and knowledge of the topography, the model requires an estimate of the vertical variation

of the wind and upper air temperature profiles in order to specify the stability. The computational domain is a rectangular box set on the earth's surface. Obstacles to the wind flow must be approximated in terms of these rectangles.

Several methods have been used to construct wind fields for the Urban Airshed Model. The appropriate method for use in a given application depends on the topography of the region and the data available (Killus et al. 1977). One method is valid only for relatively flat terrain and makes maximum use of aloft wind data. This method is not appropriate for use in areas where the terrain significantly influences the wind field. Another method was developed for use in areas with complex terrain. The inputs to this model are surface temperature field, surface roughness, elevation for each grid cell, and the wind velocity along the boundaries of the region. Surface and upper air wind measurements are also needed. The topography and boundary conditions have a dominant influence on the calculated wind field. It is therefore important that the user have a good expectation of what a reasonable wind field looks like before adjustments can be made.

The McRae et al. model uses the objective analysis technique of Goodin et al. (1980). The procedure generates mass conserving, three-dimensional winds. Unique features of the method are terrain-following co-ordinates and variable vertical grid spacing. Its mathematical formulation is very similar to the other models. Major advantages of this method are that it is computationally efficient and it allows boundary values to adjust in response to changes in the interior flow. This latter feature removes a large degree of empiricism in the model. Input data required for the model are surface level velocity measurements and upper level wind and temperature data. The influence of gross terrain features is accounted for by the use of barriers to flow during interpolation of the wind components.

The selection or development of a wind field generator requires a matching between the topography, meteorology, and observational network for the area of interest. The accuracy needed in the

interpolation routines depends on the available data. Imprecision in the measured upper air data (winds, mixing depths) makes a highly accurate interpolation procedure unnecessary. More care must be taken for surface interpolation where more measurements are available, and where there is complex terrain. All models require a certain amount of empirical input. This usually arises because direct use of the continuity equation to calculate a vertical velocity produces unrealistically large values at the top of the region. Adjustments limit this to zero, or a very small value. An operational constraint is that input data be either routinely available or readily estimated.

3.4.5 Chemistry

The chemical mechanisms from LIRAQ and McRae et al. (1982a), together with CBM III, were recently subjected to a detailed evaluation (Leone and Seinfeld 1984). Although no attempt was made to choose a "best" mechanism, problem areas were identified in all three mechanisms. In particular, the reactivity weighting of emissions used in LIRAQ was felt to be a potential source of significant problems, mainly because it cannot account for the changes in organic species composition that occur in the course of several hours of reaction. These shifts in composition are a consequence of the differing reactivities of the several species grouped together within a reactivity class.

It should also be noted that the mechanism used by McRae et al. (1982a) represents two stages of refinement of the Hecht et al. (1974) mechanism used by IMPACT and SMOG. It therefore follows that the CBM and the McRae et al. mechanism are to be preferred over the other two.

In choosing between the remaining two, the CBM is recommended as the preferred mechanism. Although both mechanisms are able to provide an adequate representation of the observed behaviour of atmospheric chemical species, the CBM has received more extensive testing, both against smog chamber results and in its use in a range

of computer models whose predictions have been tested against measured data.

It is important to note the following concerning the CBM:

1. The current release of the Urban Airshed Model does not contain the most up-to-date version of CBM.
2. The latest version of CBM, known as CBM X, is an expanded mechanism, and is likely to be too demanding computationally for use in an Eulerian model. The CBM III version of choice would therefore be
3. CBM III, as described by Killus and Whitten (1982), does not contain reactions of SO_2.
4. The detailed evaluation by Leone and Seinfeld (1984) indicated that some aspects of CBM III require refinement and updating. Specifically suggested were:
   - updating of rate constant values for reactions of DCRB (dicarbonyl group produced as intermediates) and HCHO
   - improved treatment of APRC (intermediate organic species)
   - correction of errors in the stoichiometry of radical production by photolysis of aldehydes
   - treatment of acetone as unreactive.

These appropriate refinements can be incorporated relatively easily into CBM. The need for these improvements was the primary reason why CBM was not chosen as the "best" mechanism in a recent evaluation (CSC 1985).

3.4.6 Numerical Algorithm

In this section, the different numerical schemes used for advection and diffusion by each of the four models will be critically compared. Attention will be given wholly to the profile assumptions and assembly process used to form the algebraic equation for a single grid cell. The problem of how the complete algebraic equation set is solved is not considered. This is not to suggest that the solution

procedure is unimportant in the evaluation of a numerical model. It is recognized that the choice of algebraic solver could have a significant effect on the final computational effort of the model. Rather, a lack of sufficient information in the literature, and time and resource restrictions, have made this task impractical.

A review of the literature on numerical schemes shows that much effort has been directed at developing new schemes and methods. While it may seem that a wide variety of "different" methods exist, upon close examination, the different methods show only very subtle differences. In almost all cases the major difference in the numerical schemes comes down to the use of either upwind (one-sided) or central difference approximations, or variations of these approximations to evaluate the derivatives in the transport equation. A great deal of literature has been devoted to extolling the virtues and drawbacks of these two approaches (e.g., Roache 1982); comparatively little effort has been devoted to establishing criteria by which the applicability of the methods to different classes of problems can be judged. In the work of Raithby (1976b) it is shown that guidance in the selection of a scheme is provided by how well it approximates the actual physics to which it is applied. Raithby showed that a large component of the error in the numerical solution is eliminated by following this principle.

In order to evaluate effectively the different numerical schemes used by the four models considered in this report, it is crucial that the assumptions implicit to upwind and central differencing be understood. The first part of this section explains the differences between these two approaches, and also discusses the physical situations that are best approximated by the two.

The greater part of the evaluation rests on how well the adopted numerical approximations represent the physics. Another key feature of the scheme that is evaluated is whether the scheme is conservative (i.e., does it guarantee mass conservation on both the local and global scale).

In order to simplify the explanation of the different numerical approaches it is best to consider the simple arrangement shown

in Figure 3, where we are interested in expressing the influence of the points j-1 and j+1 on j.

The central difference approach, shown by the dashed line in the figure, is equivalent to assuming that the variable ϕ varies linearly, on the local scale, between j-1 and j+1. Physically, this says that the influence of ϕ_{j-1} and ϕ_{j+1} on ϕ_j is the same, and that

$$\phi_i = \frac{\phi_{j+1} + \phi_{j-1}}{2} \quad . \qquad \text{Equation 31}$$

Physical situations where this would be a good approximation are when the transport of ϕ is diffusion-dominated. In fact, if the problem had no advection and a sufficiently fine grid, this approximation could yield an exact solution. In urban air quality models, diffusion is only dominant in the vertical direction. Because vertical acceleration is negligible, the central difference approximation for vertical diffusion is accurate. In the horizontal direction, because the effects of diffusion are small compared with those of advection, the choice of profile assumption is unimportant.

When advection dominates, with, for instance, a strong flow going from left to right, one would expect the influence of ϕ_{j-1} to exeed that of ϕ_{j+1}. Thus the linear profile assumption has the wrong physical influence on the value of ϕ_j. A more appropriate profile assumption, for this case, would be one that caused the variable ϕ_j to be represented as the "upwind" value. This reasoning is the basis for upwind differencing shown as the step profile in the figure. Physically it says that the influence of ϕ_{j-1} exceeds that of ϕ_{j+1}, and intuition would suggest that it be used in advection-dominated flows. Then

$$\phi_j = \phi_{j-1} \cdot \qquad \text{Equation 32}$$

In light of the above arguments it might be thought that the advective terms in the transport equation are best approximated by upwind differencing. This has not been the case, and it is the use of either central or upwind differences for the advection terms that has resulted in the major dilemma in numerical modelling. The problem that afflicts most methods in practice is that they will usually suffer from either non-physical, spatial wiggles, caused by

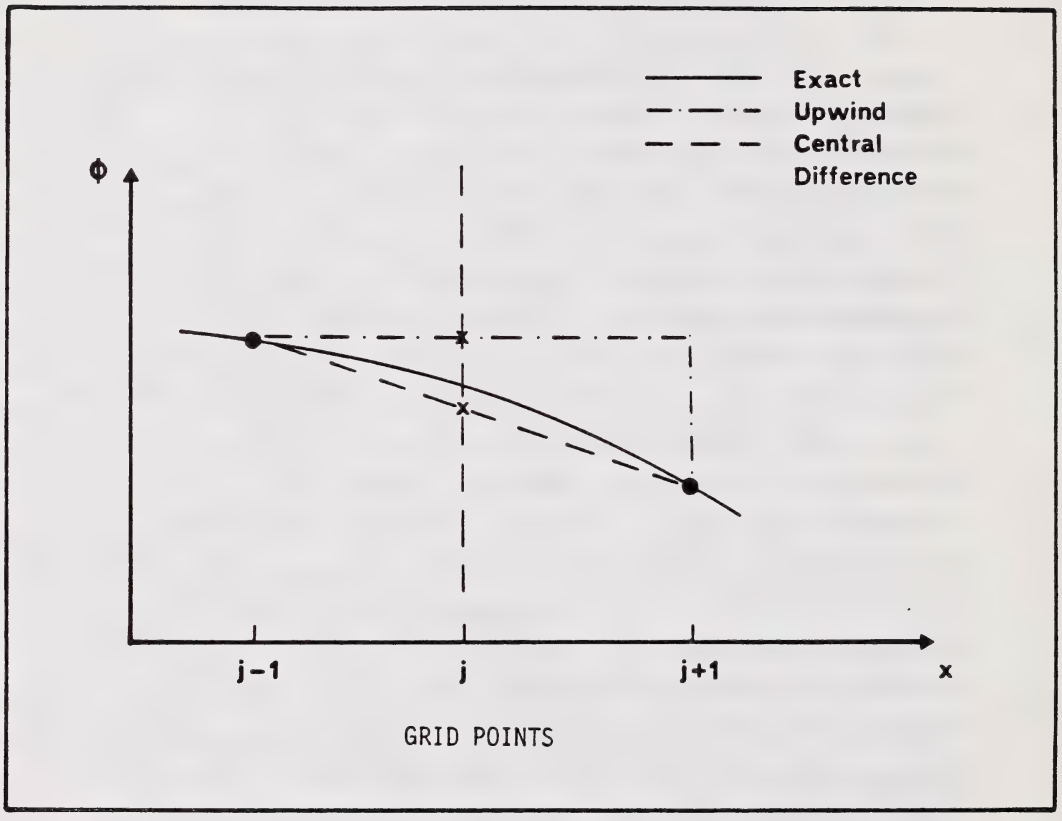

Figure 3. Illustration of upwind and central differencing.

use of a central difference profile, or false diffusion when an upwinding scheme is used.

Wiggles in the solution (equivalent to getting negative concentrations) result when central differencing is used to model the advection term. This is because the equation set that results from the linear profile assumption becomes progressively more ill-conditioned as advection dominates. Wiggles are often compensated for by "numerical smoothing" techniques, which adjust the solution to eliminate the unrealistic negative concentrations (McRae et al. 1982b).

The upwind profile assumption, it turns out, yields smooth results for either advection or diffusion-dominated flows. However, the accuracy can still be poor. The accuracy is diminished by the presence of a false diffusion. A detailed explanation of false diffusion is beyond the scope of this report. Explanations can be found in Raithby (1976), Raw (1985), and Patankar (1980). It is important to note, however, that false diffusion is not inherent in the upwind profile assumption, but results when the upwind assumption is used in certain physical situations. The basic cause of false diffusion is the practice of treating the flow between grid points as locally one-dimensional. It is a manifestation of the result that a convected variable may actually be best represented by a grid point that does not lie on the local one-dimensional profile. This is preferable when the convecting flow is not aligned with the grid lines.

As a final note, Raithby (1976a) shows that under restricted conditions, the upwind profile assumption is the most accurate profile to use. If the flow does not deviate greatly from the grid lines and the transient, source, and cross-flow diffusion is not too large, then upwinding can give good results. It is necessary to look at the wind field and emission sources in the area of interest to see if these criteria are met.

In Table 11, the finite difference forms of the simple, one-dimensional, transient, advection-diffusion equation are presented.

Table 11. Finite difference form of derivatives.

	$\frac{\partial C}{\partial t}$	$\frac{\partial}{\partial x} UC$	$\frac{\partial}{\partial x} K \frac{\partial C}{\partial x}$	COMMENTS
LIRAQ	$\frac{C_j^{n+1} - C_j^n}{\delta t}$	$\frac{u}{\delta x}(C_j^n - C_{j-1}^n)$	$(-\frac{\alpha}{2} + \frac{\alpha^2}{2}) C_{j+1}^n$ $-\partial^2 C_j^n + (\frac{\alpha}{2} + \frac{\alpha^2}{2}) C_{j-1}^n$ $\alpha = \frac{K}{\partial x^2}$	$\frac{U\delta t}{\delta x} \leq \frac{1}{2}$
IMPACT	$\frac{C_j^{n+1} - C_j^n}{\delta t}$	$(-\frac{\alpha}{2} + \frac{\alpha^2}{2}) C_{j+1}^n - \alpha^2 C_j^n$ $+(\frac{\alpha}{2} + \frac{\alpha^2}{2}) C_{j-1}$ $\alpha = \frac{u}{\delta t}$ $d = \frac{u\delta t}{\delta x}$	$\beta C_{j+1}^n - 2\beta C_{j-1}^n$ $+ \beta C_{j-1}^n$ $\beta = \frac{K}{\delta x^2}$	- time step restriction $\frac{u \cdot \delta t}{\delta x} \leq 1$
UAM	$\frac{C_j^{n+1} - C_j^n}{\delta t}$	$\frac{U_j^{-1/2}}{2\delta x}(3C_{j-1}^n - C_{j-2}^n)$ $-\frac{U_j^{+1/2}}{2\delta x}(3C_j^n - C_{j-1})$	$\frac{K_j^{-1/2}}{\delta x^2}(C_{j-1}^n - C_j^n)$ $-\frac{K_j^{+1/2}}{\delta x^2}(C_j - C_{j+1}^n)$	$\delta t_{max} = (\frac{0.5\delta x}{U_{max}}, \frac{0.5\delta x}{V_{max}})_{min}$
McRae	$\frac{C_j^{n+1} - C_j^n}{\delta t}$	$\frac{3U}{\delta x}(C_{j+1}^n \alpha_{j+1} - C_{j-1}^n \alpha_{j-1})$ α = Galerkin weighting function	$\frac{K}{\delta x^2}(C_{j-1}^n - 2C_j^n + C_{j+1}^n)$ linear finite element in vertical	- finite element formulation

Note: In C_j^n, j refers to grid location and n to time level
δt is the time increment.
δx is the space increment.

In treating the transient and diffusion terms, similarity is found in all the models. In all cases the transient terms are approximated by straight upwind differences. Diffusion terms are all approximated by central differences, but different approaches were taken in assembling the algebraic equations. For IMPACT, and for the horizontal diffusion terms in McRae et al., the Taylor series method is used to get the algebraic equations. In this approach, terms in the equations are approximated at each grid point by replacing the derivatives by finite differences that utilize values at neighbouring grid points in space and time. In the control volume approach, the method used by UAM, the finite differences are used to represent fluxes, both diffusive and advective, at the boundaries between grid points. The boundaries around the grid points define the control volume.

The greatest advantage to the control volume approach is that it guarantees that mass is conserved both at a local level (i.e., within a single control volume) and at the global level (i.e., over the entire solution domain). This property permits greater confidence in model validation, and also allows the nature of the numerical approximations to be understood and closely monitored. With Taylor series, since it is a purely mathematical approach, difficulties arising in the solutions are difficult to trace to the underlying violations of physical principles.

Greater differences are evident in the methods when the advection terms are compared. As mentioned in the preamble to this section, two different schools of thought emerge: the upwinding and the central difference approach. LIRAQ and UAM use upwind methods while the other two use central differences.

In LIRAQ, straight upwinding is used as given by a Taylor series approach. This simple method is used to save on computational effort in the version of the model that treats reactive chemistry. A more sophisticated method (SHASTA, Boris and Book [1973]) is used in the first version of LIRAQ, but this version is only used for inert species. The limited treatment of the chemistry in this model elimi-

nated it from the study. Straight upwinding, in certain flow situations, can cause significant numerical error.

The UAM, in an attempt to improve on straight upwinding, includes the influence from two grid points upwind of a control volume face. The equation is written to simulate the advective flux at a control volume face in order to maintain conservation. The extra information brought into the approximations by the extra points is felt to improve the accuracy of the solution.

The IMPACT and McRae models both use a type of central difference approximation for the advection terms. In IMPACT a quadratic interpolation (polynominal fit) is used to interpolate over $(_{j-1})$, $(_{j})$, and $(_{j+1})$. This method is known as Crowley's method (see Roache 1982). While it is true that this type of method introduces more information to the solution, it has practical drawbacks. Most notably, special methods must be used at the boundaries. In McRae et al. a finite element formulation is used to approximate the advection terms. When reduced to its basic form, this is an equally weighted central difference scheme, and the method still suffers from the negative concentration problem mentioned earlier. A valuable aspect of the finite element approach is that it affords much greater geometric flexibility, though at the cost of increased coding requirements.

A final point of note is that each of the methods is explicit, that is, the value of C_j^{n+1} is written in terms of the neighbouring Cj's at the old time n. As is shown in the final column of Table 11 this imposes a restriction on the time step that can be used. For typical model conditions this is of the order of 5 to 10 minutes.

As explained earlier, the size of the numerical error is dependent to a large extent on how well the form of the interpolation equations that are used, both in space and time, correspond to the form of the actual physical situation to which they are applied. In order to evaluate objectively different methods for use in an air quality model, they would all have to be applied to identical meteor-

ological and topographical conditions. To do this is impractical, so many studies look at much simpler situations. The paper of McRae et al. (1982b) examines a number of different upwind and central difference schemes including the straight upwind, Crowley's method, and the finite element approach. Clearly shown in these results are the effects of false diffusion in the upwind scheme, and the negative concentration problem with Crowley's and the finite element methods.

In consideration of the foregoing discussion it is felt that the best net behaviour of a numerical scheme is achieved when it is conservative and uses an upwind assumption for the advection terms. The conservation principle is desirable for its guidance in checking and interpreting model results. The preference for upwinding is because for most cases of interest, the net behaviour is improved as the wiggle problem can often make the solution meaningless or unreliable. Also for many situations, for example, in steady, non-turning winds, or in subdomains of the airshed, upwinding will give the most accurate results. Finally, while not being eliminated in numerical schemes, current research is developing modified upwind differencing schemes that greatly reduce the amount of false diffusion (Raithby 1976b; Raw 1985). It would not be a difficult task to incorporate these modified schemes into the structure of an existing upwind scheme.

3.5 SELECTION

Table 12 summarises the model component evaluations presented in Section 3.4. It contains, for each component, a ranking of the model treatments of that component, with rank one being best. In previous model evaluations (e.g. CSC 1984), this type of ranking has been followed by the allocation of a score for each component, with a total score being calculated for each model. In assembling this total score the individual component scores would be assigned different weights, depending on their importance.

However, it is clear from Table 12 that the Urban Airshed Model possesses an overall technical strength which ranks it ahead

Table 12. Model component ranking.

Component	Rank
Horizontal diffusion	1. LIRAQ 2. McRae et al. 3. UAM, IMPACT
Vertical diffusion	1. UAM, McRae et al. 3. IMPACT 4. LIRAQ
Embedded plumes	1. UAM, McRae et al. 3. LIRAQ 4. IMPACT
Dry deposition	1. McRae et al. 2. UAM 3. IMPACT, LIRAQ
Wind field[a]	1. UAM 2. McRae et al., IMPACT 3. LIRAQ
Chemistry	1. UAM 2. McRae et al. 3. LIRAQ 4. IMPACT
Numerical Algorithm	1. UAM 2. McRae et al. 3. IMPACT, LIRAQ

[a]Methods of wind field generation were not evaluated in this report. The ranking for this component is based on the availability of more than one wind field generator for UAM, and the limitation imposed on LIRAQ by the specific development of its wind field generator for the San Francisco Bay area.

of the other three models. It is therefore selected as the strongest urban scale model, without the need to allocate a score.

Several practical points also support the recommendation. First, the UAM is available from the US EPA, through the National Technical Information System, and is currently in the possession of Concord Scientific Corporation. The Model of McRae et al. (1982a), which would probably emerge as the second choice, is not currently available, and there is no intention that it will be generally released in the near future (telephone conversation with Prof. J.H. Seinfeld, August 1985).

Second, the modularity of the code means that future upgrades and refinements to the model can readily be incorporated. In particular the substitution of the most up-to-date version of CBM, including the improvements discussed in Section 3.4.4, can be achieved relatively easily.

Third, the UAM allows a number of options regarding input and output. In particular, it is possible to run the model, albeit with reduced confidence, for restricted input data. This means that control and/or emission scenarios can be initiated without being delayed by the need to collect detailed meteorological data or boundary condition data. Predictions can then be refined once these data are available.

Fourth, the UAM has been subject to extensive sensitivity tests and verification studies.

4. VERIFICATION OF THE URBAN AIRSHED MODEL

In this section, the various verification studies that have been performed on the Urban Airshed Model will be presented. Verification is a critical stage in model implementation. Successful verification provides confidence in the model as it will test for scientific vigour and consistency, demonstrate ability to predict observations, and provide insights into the link between input parameters and data and model outputs.

A complete model validation is done in three stages:

1. Basic assessment of model validity;
2. Comparison of predictions and observations for past events; and
3. Analysis of sensitivities of the predictions to uncertainties in model components.

The basic assessment of model validity refers to the essential correctness of the model in terms of its representation of the basic chemistry and physics as well as to its accuracy of numerical implementation. In essence, this is an evaluation of the individual components of the model. The UAM, in its original development (Reynolds et al. 1973) took into account the current, relevant physics. For example, the rate constants and stoichiometric coefficients used in the kinetic mechanism, that has been incorporated in the airshed model, were determined by separately validating the kinetic mechanism with laboratory smog chamber data for several hydrocarbon - NO_x systems, including auto exhaust (Reynolds et al. 1979). (Subsequent tests of the chemical mechanism have been described in Section 3.4.5). Since the original development the model has undergone a number of updates (Killus et al. 1984, Killus et al. 1977), ensuring that the most up-to-date science is being used. The basic scientific validity of the UAM was established in the component evaluation presented in Section 3.4 and need not be discussed further.

The second stage of model validation is the comparison of model predictions with observations of past events. This stage is often considered the most important in model validation. It must be

appreciated, however, that it is difficult to ascertain the cause of discrepancies between predictions and observation. There are many points at which errors can enter a complex Eulerian model. For example, the errors could be due to inadequacies of input data such as emission inventories, or incorrect representation of the basic physical and chemical processes. Guidance in trying to understand the causes of discrepancies between predictions and observations is provided by sensitivity studies. This is the final stage in model validation.

A sensitivity study requires that the model be analysed to determine the input parameters, input data, and model variables to which the model is most sensitive. Also, it requires that the sensitivity of the input to perturbations in the input parameters be assessed. By combining the output variations with estimates of the levels of uncertainty associated with each input parameter and variable, this analysis will indicate how much of the overall uncertainty of the model output is associated with the individual uncertainty in each model input.

In the following two sections the different comparison and sensitivity studies which have been performed on the UAM will be discussed.

4.1 COMPARISON STUDIES

The UAM, since its development, has been evaluated against a number of different pollution episodes. The model was initially applied to pollution episodes over Los Angeles on six separate days in 1969, each day exhibiting somewhat different meteorological conditions and smog severity (Reynolds et al. 1974). Runs were made for the 10-hour period between 0500 to 1500 hours. Separate comparisons were made to CO (inert species) and for hydrocarbons, nitrogen oxides, and ozone.

Because it is an inert species, comparison of model predictions with measurements of CO concentration provided a validation of the meteorological facets; in particular the treatment of the winds and the inversion, the numerical integration scheme, and portions of

the source emissions inventory. CO predictions were compared for the average concentrations in each four square mile area that contained a monitoring station. It was found that CO was underpredicted for those monitoring stations located in the vicinity of a busy roadway. This led to the development of a microscale model which predicted local corrections for model predictions on grid squares where sub-grid effects were significant.

Validation for hydrocarbons, nitrogen oxides, and ozone consisted of two parts; namely, validation of the kinetic mechanism both in the absence and presence of transport processes. The first part refers to the comparison of the predictions of the kinetic mechanism with laboratory smog chamber data. The second part refers to the comparison of the predictions of the full airshed model with monitoring data. Consistency was shown in the predictions. All results were at least qualitatively in agreement with observations, and in many cases good quantitative agreement was also achieved.

Weaving et al. (1979) tested the suitability of UAM to simulate photochemical phenomena in European cities. Specifically, the model predictions were compared against measurements obtained in the City of Turin, Italy during a day when photochemical activity was observed. Reactive hydrocarbons (HC), NO, NO_2, O_3, and CO were predicted over the city from 0500 to 1600 hours. Certain model refinements were necessary before the model could be applied to Turin. The vertical diffusivity was modified to incorporate the effect of thermal convection on the mixing processes because winds are very light in Turin and this type of mixing dominates during sunny summer days. The emission algorithms were also modified to allow for the effect of the different driving cycles encountered in the city.

It was found that maximum predicted CO concentrations were in satisfactory agreement with observations. The average spatial and temporal distribution of hydrocarbons compared well with observations although there was some disparity between the magnitudes and timing of the peak concentrations. A significant portion of the discrepancy

found in the predictions was attributed to a lack of reliable measurements outside of the solution boundaries.

The UAM was used by Builtjes et al. (1980) to predict pollution concentration levels for an area covering the Netherlands and its surroundings. The modelling region was chosen large enough to include important industrialized areas in Belgium and Germany. The concentrations in the area under consideration are thus predominantly determined by emissions inside the modelling region. This reduces the model sensitivity to background concentrations.

The model was applied to the simulation of the photochemical episode of 7 and 8, June 1976. The 310 x 230 km area was divided into 10 x 10 km^2 grid cells with five vertical levels.

The agreement between measured and calculated concentrations of O_3, and to a lesser extent of NO_2, was found to be remarkably good, both in terms of distribution patterns and peak values. Also carried out as part of this study was a sensitivity analysis which will be discussed in the next section.

Stern and Scherer (1982) applied UAM to the Rhine-Ruhr area in the Federal Republic of Germany. One of the main features of this area is the complexity of the wind conditions induced by the complexity of the terrain. Therefore, special emphasis was given to the preparation of the three dimensional wind field.

The photochemical smog episode of 1976 June 22 to 27, was simulated. A region of 160 x 176 km^2 including all major industrial sources was chosen as the modelling region. The region was divided into 22 by 20 grid cells of 8 x 8 km^2 in the horizontal and five cells in the vertical. Because of the complexity of the wind field, two different methods were used, one based on interpolation of surface winds (objective analysis technique), the other on a prognostic meso-scale model (Mahrer and Pielke 1977). The calculated concentrations of O_3, NO, and NO_2 utilizing both of the wind fields were compared with measurements.

Predicted O_3 concentrations compared with the observations of four urban and two rural stations were in rather good agreement, although, calculated peak ozone values showed a tendency toward over-

estimation. Also well predicted was the spatial distribution (ozone plumes) emanating from the maximum hydrocarbon emission area in the centre of the modelling domain. This provides confidence in the wind field modules which are responsible for the advection of pollutants.

Overall, the UAM results were in reasonably good agreement with measured ozone values at urban sites using both wind field models. For rural sites, the model tends to underpredict the ozone concentrations during the night. The pattern of diurnal variation was simulated quite well. Calculated peak ozone concentrations showed a tendency toward overprediction. The model was found to be less successful in reproducing measured NO_x concentrations since the NO_x measurements are strongly influenced by local sources. The underestimation was attributed to the averaging properties of the grid cells.

Two comparison studies that were performed including UAM are those by Schere and Shreffer (1982, 1983). The purpose of this research was to determine the accuracy of four photochemical air quality simulation models using data from the Regional Air Pollution Study (RAPS) in St. Louis. In the first study, UAM was evaluated against a box model, a Lagrangian model, and the LIRAQ Eulerian model. Emphasis was placed on the ability of the models to reproduce the maximum one-hour ozone concentrations observed on 10 days and selected from nearly two years of data. In the second study, LIRAQ was dropped from the evaluation and the observations were increased to 20 days.

The Urban Airshed Model was found to match predictions as well as, or better than the other models. Consistent with the findings of the earlier comparison studies, fair agreement was found in the ozone distribution patterns, but correlation was relatively poor between peak values.

A final comparison study is that of Cole et al. (1982), in which the UAM was compared against the Regional Air Pollution Study (RAPS) of St. Louis. Twenty days (11 from 1975 and 9 from 1976), each with high measured ozone, and different meteorological regimes were

chosen for comparison. Three hundred horizontal grid squares, each 4 x 4 km^2 were used.

A comprehensive comparison which included accuracy of peak predictions, overall accuracy, overall precision, and the ability of the model to reproduce spatial and temporal patterns of variation were performed. As in the previous studies, when the predicted maxima were compared with the observed maxima for the same time and location, correlation was relatively poor. However, when comparison was made between peak observations and the highest predicted value without regard to time or location, agreement was much better (within 30%). This suggests that the apparent discrepancy is not due to the failure of the model to generate the observed peak value, but from displacement of the peak in time and space.

The model represents the temporal variation of ozone quite well, and was able to simulate the diurnal pattern found in the observed data: low values in the morning, a build up toward afternoon, and decreasing values toward evening. The correlation of spatial variation was not as high as for the temporal variation. The latter correlation was found to vary considerably from day to day. For some days the model does reasonably well in replicating general patterns, for other days strong discrepancies exist.

Model evaluation has been the subject of a number of studies (Demerjian 1984; Downton and Dennis 1985; Dennis and Downton 1984; Fox 1981). These studies have looked at different statistical measures for evaluating the performance of urban air quality models. Downton and Dennis (1985) demonstrated the importance of designing an evaluation to take into account the way in which the model will be used in regulatory practice, and then choosing performance measures on the basis of that design. Model use is important in considering that the choice of performance measure affects outcome. This was shown to be the case when the different methods of comparing peak values were presented. Recall that each of the studies showed relatively poor correlation when peak values were compared at fixed time and space locations. When peak values were compared without regard to time and

location, correlation was quite good indicating that the model performs reasonably well in characterizing the magnitude of peak values at some location within the solution domain.

In summary, the studies reviewed demonstrate that UAM is able to estimate peak observed concentrations with a reasonable degree of accuracy; prediction of time and location of the peak is less reliable but is at least as good as that of other models. The model represents the temporal variation of pollutants quite well, but its ability to reproduce spatial variation varies. Comparison of NO_x prediction/observed values demonstrated the importance of a sub-grid model. The model would typically calculate ambient concentrations averaged over the volume of a grid cell. This spatial resolution is not sufficient to predict the concentrations in streets close to traffic. First, the proximity of sources results in considerably higher levels in the street. Second, the very short atmospheric transport time of the pollutants and the very fast concentration fluctuations may result in important deviations from the photostationary equilibrium. The freshly emitted NO will result in lower O_3 levels and higher NO and NO_2 levels at short distances from the roadway. A description of these curbside levels would require application of a different type of model.

The comparison exercises indicate that the model is sufficiently accurate for use in control strategy simulations. However, there is still some uncertainty associated with the predictions. Model validation requires sensitivity tests to determine how much of the overall uncertainty of the model output is associated with the individual uncertainty in each model input. In the following section, various sensitivity studies that have been performed on the UAM will be described.

4.2 SENSITIVITY STUDIES

The basic purpose of sensitivity studies is to determine the relationships between the input data and the output concentrations. The determination of the model response to changes in input parameters

and functions is particularly important because of the non-linear nature of the model.

The sensitivity of the UAM to various input functions was tested by Liu et al. (1976), Peterson and Demerjian (1976), and Dunker (1980). These studies attempted to determine the range over which model inputs could be varied to get a linear response in output. It was found that $\pm$ 20 to 30 percent changes in initial conditions, emission rates, or boundary conditions produce concentration changes approximately linear in output variable even though the model contains non-linear chemical reactions. A 20 percent change in speed produced a linear change in output. Any change in wind direction or vertical diffusivity produced a non-linear change in output. The model was not sensitive to changes in horizontal diffusivity.

Builtjes et al. (1980) performed sensitivity studies on the hydrocarbon emissions and boundary conditions. They found that increasing the hydrocarbon levels at the boundaries resulted in increases in O_3. Because of the absence of large sources of hydrocarbons, rural areas were found to be much more sensitive to the boundary conditions than urban areas.

It was estimated that emissions had an overall uncertainty of 30 percent. By varying NO_x and HC emission by $\pm$ 30 percent no significant change in O_3 was observed. There was a clear effect on NO concentrations and to a lesser extent NO_2 levels.

Cole et al. (1982) conducted sensitivity tests to determine how the UAM predictions of ozone respond to changes in hydrocarbon emissions. To establish the response over a wide range reductions of 5, 17, 42, and 75 percent and increases of 17 and 63 percent were tested. The tests were run for three different days. Because of the different meteorology, the changes on all three days were different, but in all cases the changes were less than 1:1, i.e., a 17 percent reduction in HC resulted in a less than 17 percent reduction in O_3. It was also found that with greater degrees of hydrocarbon reduction, the location of the predicted peak zone is displaced downwind and tends to occur later in the day.

Additional sensitivity tests were conducted in order to assess how changing NO_x emissions would affect the model's ozone/hydrocarbon response. Uniform increases and decreases of NO_x emissions were coupled with a 42 percent reduction in HC emissions for the three test days. The results indicate that decreases in NO_x emissions (by 20 percent from the base case) result in a lessening in the effectiveness of HC emission reduction in decreasing peak ozone concentration.

The final sensitivity study that will be discussed is that of Seigneur et al. (1981). In this study, 22 sensitivity cases were run in terms of the amount and quality of meteorological, air quality, and emission data as well as modifications of the model gridded structure. This study attempts to determine the extent to which the amount and quality of data input to complex models can be reduced from the level of current practice without substantially degrading the accuracy and reliability of model predictions. A knowledge of model sensitivity to the level of detail of input data provides one means for estimating data needs and resource requirements. The studies were carried out for the Los Angeles basin because of its extensive database and because simulation results proved to be quite satisfactory. Calculations for all base case runs were made on a 5 x 5 km^2, 34 x 20 horizontal grid with four vertical layers.

Twenty-two different sensitivity tests were made on the meteorological, air quality, and emissions data, and on the model grid structure. The sensitivity tests consisted of reducing the input data detail. For example, the number of upper and surface air quality and meteorological stations used to specify initial and boundary conditions, and the wind field was reduced. In another case, the detail in emissions was reduced by basing point source emissions on annual averages rather than a diurnal temporal profile. A complete listing of all the sensitivity runs can be found in Seigneur et al. (1981) and Tesche et al. (1981).

The most significant changes in concentration (15 to 45 percent) resulted from reductions in the upper air meteorological

data. The model was highly sensitive to the upper air data detail because of the wind field module used. The wind field is obtained from the solution of a parameterized, three-dimensional boundary value problem. Therefore, the model is more sensitive to atmospheric data at the boundaries of the airshed and at the top of the mixing layer than a wind model would be if it were based on surface data interpolation by inverse weighting.

The base case estimates of initial hydrocarbon concentration were calculated from total hydrocarbon concentrations by means of a regression formula obtained from gas-chromatography atmospheric measurements. For the sensitivity study, the initial hydrocarbon concentration was assumed to be seven times the concentration of nitrogen oxides. Thirty to forty percent changes in O_3 were found. This large perturbation suggests that the definition of the initial concentrations of reactive hydrocarbons is an important model input.

The next largest perturbation was found with the grid refinement studies. Reducing the vertical structure from four to one layer resulted in a 20 to 37 percent change in ozone. Grid reduction from four to two layers had relatively little effect on model performance. This simplication could be used to reduce computational costs without greatly affecting the accuracy of the simulations. However, the use of a single layer leads to large deviations in model predictions. This is due in part to the fact that elevated emissions are entrained outside of the single layer model, whereas in the multilayer case, the NO_x emission released in the inversion layer can be re-entrained later into the mixing layer.

A courser grid of 10 x 10 km^2 produced a 20 percent change in ozone. All other perturbations were less than 15 percent. Reductions in the surface meteorological data affected mixing depths, wind direction, and wind speeds. Some deviations in ozone levels were observed, but they were not as large as those caused by the upper air meteorological data. Reductions in air quality data did not greatly affect model predictions, nor did a less sophisticated emission inventory for mobile source emissions. Changes in the temporal

resolution of point and area source emissions did not lead to any major perturbations in the air quality simulations.

To obtain a ranking of data needs, the ozone variability measurements were weighted by the uncertainty in the input and by the cost of obtaining the data. From this, a sensitivity uncertainty index was defined. This allowed ranking of data needs in terms of the sensitivity of the model predictions to the amount of input data, the costs of data acquisition, and the uncertainties in the air quality model input variables. The rankings suggest that a mobile source inventory should be obtained because of the relatively low cost involved and because of the reasonable accuracy of mobile source emission rates. Upper air meteorology and the initial conditions for reactive hydrocarbons are ranked high, despite the relatively high cost of large monitoring program. Spatial resolution of area sources, upper air pollutant concentration data, detailed hydrocarbon speciation, and a detailed point source inventory are of a similar value to model performance. The importance of surface meteorology is of the same order.

Because detailed specification of transportation patterns is a rather expensive task, the need for such input data receives a very low ranking. Since quantification of the temporal distribution of stationary source emissions is also expensive to obtain and has little effect on model performance, it too, receives a low ranking.

It must be remembered that some of the results obtained by Seigneur et al. (1981) are dependent on the length and meteorology of the simulation period and on the site. Therefore, their results should not be considered conclusive of the performance of the UAM. Rather, the method should be seen as a procedure for defining input data needs and the results should be considered as an illustration of the method.

The generality of the sensitivity simulation results presented in this section is limited because of the dependence of the model on the specificity of the location, the atmospheric conditions, and the modelling conditions (e.g., length of simulation time and type

of wind field model). However, the general nature of the methods provide a useful framework for the development of further sensitivity studies in other areas.

5. INPUT AND RUNNING REQUIRMENTS

In order to run a Eulerian grid model, input data are required in the form of initial and boundary conditions and the spatial and temporal distributions of wind and pollutant sources. At first inspection, it would seem as if a transient, three-dimensional model would require the support of an extensive meteorological and air quality observational network. While it is desirable to have a large observational network with which to provide initial and boundary conditions, reliable estimates for wind field generation, and data that can be used to validate model runs, it is not a necessity for the UAM. An attribute of this model is that it has a great deal of flexibility in the amount and form of the input data that it will accept, although confidence in the model predictions is obviously closely linked to the accuracy and completeness of the input data, as has been discussed in the previous section.

The collection and processing of the available meteorological, air quality, and emissions data, as well as other information such as that pertaining to the topography and land use of the area, is very site specific. The type, amount, and form of this data will depend on what is being measured, the state of the observational network, and the type of instrumentation being used. Recognizing this, the UAM is equipped with a series of programs that create the appropriate data files in a form suitable for input to the model.

The different methods that are available have different data requirements. The choice of method is determined by the user on the basis of the amount of data available and the general characteristics of the physical and chemical phenomena that influence the pollutant concentrations in the region. The choice of the data handling method should make the best possible use of available data and knowledge. In light of these comments, if the existing subroutines for preparing inputs are not best suited for a particular data set, allowance is made for a more suitable procedure, developed independently of the UAM by the user, to be implemented in the model.

The following discussion describes the complete input data requirements for the model and the type of data needed as input for the existing preprocessor programs. A comprehensive presentation of these requirements can be found in the UAM user guide (Ames et al. 1982).

5.1 METEOROLOGICAL INPUTS

Meteorological inputs include the three-dimensional wind field, parameters needed to estimate stability, mixing height distributions, and topographical features. The level of detail required in each of these variables is not the same. Table 13 shows the spatial and temporal dependence of each of the meteorological variables required by the UAM. A variable with temporal dependence requires that its value be supplied to the model in an appropriate way at each time step in the simulation. Spatial dependence can be vertical, horizontal, or both. Vertical dependence calls for the variable to be specified at each grid point between the ground and the top of the solution domain. Horizontal dependence requires specification in just the horizontal plane. This can be done either at the ground, the mixing height, or the top of the solution domain, as appropriate.

As was mentioned earlier, a number of different options exist, allowing different levels of detail in the specification of these parameters. The different methods that are available are summarized in Table 14. Again, the choice of method must be directed by the physical situation being simulated and the available data. It should be noted that, in practice, the model can be run without any measured data. In this case, the user would use either the Constant or Grid Value routines and supply a reasonable estimate of the field.

As can be seen in Table 13, the wind field has a fully three-dimensional and temporal dependence. The different approaches available in the UAM are given in Table 14, and were also discussed in Section 3.3.4. Mixing heights and the top of the solution domain must be estimated in the horizontal plane and must be supplied at the

Table 13. Meteorological inputs required by UAM.

Meteorological Variable	Dependence		
	Spatial		Temporal
	Horizontal	Vertical	
Wind	✓	✓	✓
Surface Temperature[a]	✓		✓
Surface Roughness	✓		
Land Use[a]	✓		
Mixing Height	✓		✓
Top of Solution Domain	✓		✓
Atmospheric Pressure			✓
Relative Humidity			✓
Temperature Gradients above and below inversion			✓

[a]Optional

Table 14 Input file methods.

Method	Description	Requirements
Horizontal		
• Constant	Constant value everywhere	Input by user
• Grid Value	Constant for each surface location	Input by user
• Interpolation	Individual grid values determined by interpolation of station values • weighted distance • Poisson • Linear	Measured station values, station locations
• User-Supplied	User-supplied routine	Dependent on routine
Vertical		
• Constant	Values in vertical cell are equal to ground level value	Ground level values
• Extrapolation	Vertical profile dependent on ground level value	Ground level values
• Interpolation	Interpolation between ground level and top of region value, as for horizontal case	Ground and upper level value
• User-Supplied	As for horizontal	As for horizontal
• Temporal		Values at beginning of each average time step (usually an hour)

beginning of each average time step (one hour). For solution time steps less than the average, the heights are determined by linear interpolation. Also, the option exists of specifying the mixing and solution domain heights independently, or of relating them (i.e. mixing height will be a fixed fraction of the solution domain height).

Surface roughness and land use have only horizontal dependence, while surface temperature has horizontal and temporal dependence. Note that these are optional routines. If they are not used, a homogeneous value is used. Surface roughness is used in calculating diffusivity profiles. The land use factor is used in calculating deposition velocity, and the temperature field is used in calculating the temperature-dependent rate constants for the chemical reactions.

Finally, the meteorological scalars (atmospheric pressure, relative humidity, and temperature gradients) need only be supplied at each time step. Their values are assumed to apply at all locations in the grid.

5.2 EMISSIONS DATA

Because of the variability in pollutant emissions, no general-purpose routine exists in UAM for the processing of emission data. The file that exists allows the user to tailor a routine to match the particular area requirements. For ground level emissions, time-varying ground level emission fluxes must supplied as either point, area, or line sources. Horizontal dependence can be specified with the Constant or Grid Value methods (Table 14).

The routine that calculates elevated point source impact requires the stack location and height, and the emitted species, and either the pollutant flow rate or stack diameter and velocity. Also needed to calculate plume rise is the stack temperature. A summary of these requirements is found in Table 15.

Emission rates are typically required for those chemical species that participate in the reaction mechanism and a number of inert species. Although the Carbon Bond Mechanism used in the UAM

Table 15. Emission inputs required by UAM.

Source Type	Description	Requirements
• Ground Source	Time-varying, ground level emission fluxes	User-supplied, point, areal, line source, species Constant or Grid Value methods
• Elevated Source	Time-varying, elevated point sources	Location, stack height, species, stack diameter, stack temperature, emission flow rate or velocity

has specialized requirements regarding the specification of organic reactivity, emission inventories designed for use with the UAM (Engineering Science 1980, 1982) have resolved organic compounds to ethene, other alkenes, carbonyl compounds, alkanes, and aromatics. Other reactive species are NO and NO_2. Typically CO would be included as an inert species.

The emission rates should preferably be tabulated on the same spatial resolution as is used in the model, i.e., normally on a 5 x 5 km grid.

5.3 CHEMISTRY INPUTS

The chemistry inputs for the non-photolysis chemical reactions differ from the other inputs because they are specific to the mechanism rather than being dependent upon the region and the date of the simulation. The rate constants and activation energy for each non-photolysis chemical reaction must be input to the model.

For the photolysis rate constants a little more information is used. The UAM requires that the NO_2 photolysis rate be specified as constant at set times, usually one-hour intervals. Interpolation is used to calculate the photolysis rate constant at each integration time step, and other photolysis rate constants are assumed to be proportional to this value.

5.4 INITIAL AND BOUNDARY CONDITIONS

Estimates of the spatial distribution of each pollutant species at the start of the simulation and their background levels (levels outside the solution domain) are required for the specification of initial concentration fields, and boundary conditions.

Table 16 summarizes the type of initial and boundary conditions, and Table 17 contains their running requirements. The initial concentration has to be specified for each grid cell and for each species. Because measured air quality data is generally limited, the user will normally make maximum use of the different methods available in the UAM for interpolating and extrapolating data.

Table 16. Initial and boundary conditions.

Initial	$C_i(x,y,z\ t_o)\ Fi(x,y,z)$	
Boundary		
$Z = h(x,y)$	$-K_v \cdot \frac{\partial C_i}{\partial Z} = Q_i(x,y,t)$	
$Z=H(x,y,t)$	$(V \cdot C_i - K_N \frac{\partial C_i}{\partial Z}) = V \cdot gi(x,y,z,t)$	V into domain
	$-K \frac{\partial C_i}{\partial Z} = 0$	V out of domain
	$V - ui - vj + (w - \frac{\partial H}{\partial t})k$	
Horizontal	$UC_i - K \frac{\partial C_i}{\partial x} = U \cdot gi(x,y,z,t)$	U into domain
	$- K \frac{\partial C_i}{\partial x}$	U out of domain
	same for other horizontal direction	
	$gi(x,y,z,t)$ = concentration outside domain	
	$Q_i(w,y,t)$ = ground emission flux	

Table 17. Initial and boundary condition input required by UAM.

	Description	Requirements
Initial	Initial concentration at each grid point	- use horizontal and vertical methods (Table 14)
Boundary		
Z=h(x,y)	Mass balance at surface	- ground source emissions
Z=(H(x,y,t)	- mass flux continuous at upper boundary	- concentration at top of region
	- negligible diffusion at top	- velocity at top of region
Horizontal	- mass flux continuous across boundary when flow is into the airshed	- concentration at region boundary
	- negligible diffusion when flow is out of the airshed	

Depending on the available data and the importance of the particular pollutant species, different methods can be used. Possibilities include using exactly the same concentrations for the upper layers as for the surface layer, or extrapolating a vertical profile that is scaled according to the surface concentration, or that is interpolated according to the surface concentration and the boundary concentration at the top of the region. If measurements for some pollutants are not available, they can be specified to have some background level.

The boundary conditions express mass balances at the region boundaries. These specify the concentration of pollutants in the air entering the modelling region through the side as a result of horizontal advection, or through the top of the region as a result of vertical convection and entrainment caused by changes in the region height. If air is flowing out of the modelling region, then the material in the cell adjacent to the boundary is allowed to advect out of the region.

Again, all of the horizontal and vertical specification routines in Table 14 can be used in specifying the boundary conditions. The conditions can also be allowed to vary in time. The time scale over which the boundary conditions vary is usually an hour, but this can be changed to fit the particular application.

Concentrations at each boundary, and subregions of the domain boundaries can be specified independently. This is particularly useful if there is a large plume upwind of the solution domain. In such a case, the concentration of pollutant as it encounters the airshed boundary can be estimated and assigned to the appropriate grid cells. If the boundary concentrations are not known, they can be assigned a nominal value.

5.5 HARDWARE REQUIREMENTS

The actual computer resources required by the UAM are not precisely known. Because they are dependent on the simulation time, the number of grid points used, the size of the grid cells, and a number of other factors, one can only obtain estimations by looking

at the requirements of a typical simulation. Wada et al. (1979) reported that the UAM, run for a 14-hour simulation with a 25 x 25 horizontal grid and four vertical layers, required 20 minutes of machine time on a CDC 7600. Nearly one million bytes of memory were required.

5.6 DATA AVAILABILITY

A survey was made of data availability for Edmonton and Calgary to determine how closely the requirements of the UAM, as discussed above, can be met. The results of the survey are summarized in Tables 18 and 19.

It is clear from these tables that the meteorological and chemical concentration data for these two cities are sparse, particularly for Calgary. Although the model can be run with minimal input data, the credibility of the results obtained depends critically on the quality of the inputs. It will therefore be necessary to supplement the available measurements. In addition, ambient concentration measurements will be required for at least one intensive period to allow the model to be tested and validated.

Emission inventories have recently been compiled for both Edmonton and Calgary (Truch 1985). The spatial resolution is to a 1 x 1 km grid, and data was collected for the five criteria pollutants: SO_2, NO_x, CO, particulate matter, and hydrocarbons. These inventories will form a suitable basis for the emission data files required by UAM, but further work will be necessary. Specifically, speciation of NO_x to NO and NO_2, and hydrocarbons to the appropriate reactivity groupings is required. In addition, temporal patterns of emissions must be provided, including dependence on season of year, day of week, and hour of day. An additional point to consider is that the inventory domains may not coincide completely with the modelling domains, so that supplementary data collection may be required.

The inventories have been stored on magnetic media in Lotus 1-2-3 spreadsheet format.

Table 18. Meteorological Observing Stations in the Vicinity of Edmonton and Calgary.

OPERATOR/ID#	NAME	LOCATION LAT °'N LONG °'W	ALTITUDE (m) a.m.s.l.	MOST RECENT PERIOD OF CONTINUOUS OBSERVATION	SURFACE WIND (10m, unless indicated)	UPPER AIR OBSERVATION	METHOD FOR CALCULATING STABILITY	MIXING HEIGHT OR ABILITY TO CALCULATE	CLOUDS BASE/AMOUNT HEIGHT	PRECIPITATION	DRY BULB TEMPERATURE	HUMIDITY	RADIATION/ SUNSHINE	COMMENTS
AES/3011138	CALMAR WEST	53 17, 113 55	732	1970/01→						✓ 24h				
AES/3018B03 ALBERTA ENV	EDMONTON CBC (TOWER)	53 31, 113 16	732	1974/08-1980/02	92M									
AES/3012205	EDMONTON INT'L A	53 18, 113 35	715	1972→	✓		PGT		✓	✓+ rate	✓	Dew Point	Sunshine	
AES/3012208	EDMONTON MUNICIPAL A	53 34, 113 21	671	1975/08→	✓		PGT		✓	✓+ rate	✓	Dew Point	Sunshine	
AES/3012210	EDMONTON NAMAO A	53 40, 113 28	688	1964/10→	✓		PGT		✓	✓+ rate	✓	Dew Point	Sunshine	
AES/301222F	EDMONTON STONY PLAIN	53 33, 114 06	766	1966/02	✓+ mileage	✓ radiosonde	UA sounding	UA sounding		✓	✓	✓	Global, Sky, Net	
AES/3018B8F ALBERTA ENV	EDMONTON TELEPHONE (TOWER)	53 34, 113 34	673	1974/08-1977/08	✓+ 92m						✓+ 92m			
AES/3012230	EDMONTON WOODBEND	53 29, 113 45	671	1973/11→						✓ 24h	Max, Min			
AES/3012659	FORT EDMONTON	53 31, 113 34	628							✓ 24h	Max, Min			
AES/3012295	ELLERSLIE	53 25, 113 33	694							✓+ rate	Max, Min		Sunshine	
Dept. of Geography U. of Alberta	"	"	"	1975	✓ ✓+ 2m					✓	Max, Min		Global	Contact Mr. P. Hof (403) 432-5406
Dept. of Mech. Eng. U. of Alberta	"	"	"		✓ (hourly)						✓ (hourly)			Also various radiative fluxes. Data recorded on computer as hourly averages
NAPS PCD/EWMU	"	53 19	687	1978→	✓+ 20m	Minisonde soundings 4 times daily Jan, Apr, Jul, Oct, (1978-83)	Sigma-theta Sigma w bulk Richardson # Gradient Richardson # M.O. length Radiation	DAS Minisonde		Event monthly	8m ΔT 8-18m		Global Net	Heat flux, Vertical wind, Δσ, Δθ Contact, J. Godin, (403) 988-5166
NAPS ALBERTA ENV PCD/EWMU	EDMONTON RESIDENTIAL MONITORING UNIT	53 36, 113 32			✓									Contact, J. Benoit (403) 427-5893
NAPS PCD/EWMU	EDMONTON INDUSTRIAL MONITORING UNIT	53 33, 113 22			✓									Contact, K. Luklnuk (403) 427-5893

...."Continued"

Table 18.Concluded.

OPERATOR/ID#	NAME	LOCATION LAT °'N	LOCATION LONG °'W	ALTITUDE (m) a.m.s.l.	MOST RECENT PERIOD OF CONTINUOUS OBSERVATION	SURFACE WIND (10m, unless indicated)	UPPER AIR OBSERVATION	METHOD FOR CALCULATING STABILITY	MIXING HEIGHT OR ABILITY TO CALCULATE	CLOUDS BASE/AMOUNT HEIGHT	PRECIPITATION	DRY BULB TEMPERATURE	HUMIDITY	RADIATION/ SUNSHINE	COMMENTS
AES/3031A0Q6	CALGARY ELBOW VIEW	51 01,	144 12	1128	1967/08→										
AES/3031093	CALGARY INT'L A	51 06,	144 01	1084	1969/07→	✓				✓	✓+ rate	✓	Dew Point	Sunshine	
AES 3031A0Q ALBERTA ENV/ CAMU NAPS	CALGARY TOWER BONNY-BROOK	51 01,	114 01	1029	1974/08-1980/05	✓+ 92m		Bulk Richardson #			✓ 24hr	✓+92m			Contact, D. Bensler (403) 297-8272
AES/3031676	COCHRANE	51 13,	114 26	1280	1961/08→						✓ 24hr				
AES/3021950	CROSSFIELD	51 25,	114 10	1128	1971/05→						✓ 24hr	Max, Min			
AES/3033242	HIGH RIVER RADIO	50 35,	113 54	1039	1980/06→						✓ 24hr	Max, Min			
AES/3055120	PESKISKO	50 22,	114 25	1439	1914/05→						✓ 24hr	Max, Min			
AES/3036641	TURNER VALLEY RS	50 40,	114 21	1219	1972/06→ (Summer Only)						✓ 24hr	Max, Min			
AES/3036652	U. OF CALGARY	51 05,	114 08	1112	1977/02→						✓ 24hr	Max, Min			
DEPT. OF GEOGRAPHY U. OF CALGARY		"	"	"	Raw data from 1964	✓	Summer Rawinsonde (Mid June-Aug. 1) →		→		✓	✓	✓	Radiometer for some periods	Rawinsonde part of hail program. Data has been card punched up to ≈ 1976/77. Some processing into means carried out. Contact, T. Rhodes (403) 284-6065.
DEPT. OF PHYSICS U. OF CALGARY	SPRINGBANK AIRPORT & OTHER LOCATIONS				Continuous Winter 1984/85 Winter 1983/84 at Calgary Int'l				DAS						Inversion height data from Calgary Int'l. Winter 1983/84. Contact Dr. T. Mathews/Dr. Harrison (403) 284-6337.
NAPS ALBERTA ENV. PCD/CAMU	CALGARY RESIDENTIAL MONITORING UNIT	51 05,	114 08			✓									Contact, T. Speckman (403) 261-8263

PGT - Pasquill-Gifford - Turner
UA - Upper Air Sounding
DAS - Doppler Acoustic Sounding
NAPS - National Air Pollution Surveillance Program

Table 19. Air Quality Monitoring Network Summary for Calgary and Edmonton

Station Name and Number	Location	Operated By	Type	Operation/ Frequency	Parameters Monitored: Oxidants O_3	NO_x	Particulate	CO	SO_2	Other
CRMLU 90222	39 Street and 29th Avenue N.W.	NAPS	Residential		✓	✓	✓	✓	✓	Soiling Index HC
CDM' 90227	611-4th Street	NAPS	Downtown		✓	✓		✓	✓	
CIMU 90218	45 Avenue and 18A Street S.E.	NAPS	Industrial		✓	✓		✓	✓	
50A	Crossfield - SE trailer	AIAAM	Industrial	12 mth/year					✓	Sulphation H_2S wind
50B	Crossfield - SE trailer	AIAAM	Industrial	12 mth/year					✓	Sulphation H_2S wind
51	Harmattan	AIAAM	Industrial	12 mth/year					✓	Sulphation H_2S wind
52	Lone Pine Creek	AIAAM	Industrial	6 mth/year					✓	Sulphation H_2S wind
53	Okotoks	AIAAM	Industrial	12 mth/year					✓	Sulphation H_2S wind
54	Lone Pine Creek	AIAAM	Industrial	9 mth/year					✓	Sulphation H_2S wind
55	Quirk Creek	AIAAM	Industrial	12 mth/year					✓	Sulphation H_2S wind
56	Carstairs	AIAAM	Industrial	6 mth/year					✓	Sulphation H_2S wind
57	Morley	AIAAM	Industrial	2 mth/year					✓	Sulphation H_2S wind
58	Cochrane-Wildcat Hills	AIAAM	Industrial	12 mth/year					✓	Sulphation H_2S wind
59A	Balzac-SE trailer	AIAAM	Industrial	12 mth/year					✓	Sulphation H_2S wind
59B	Balzac-NE trailer	AIAAM	Industrial	12 mth/year					✓	Sulphation H_2S wind
60	Burnt Timber	AIAAM	Industrial	12 mth/year					✓	Sulphation H_2S wind
61A	Jumping Pound NE trailer	AIAAM	Industrial	12 mth/year					✓	Sulphation H_2S wind
61B	Jumping Pound NW trailer	AIAAM	Industrial	12 mth/year					✓	Sulphation wind
61C	Jumping Pound SE trailer	AIAAM	Industrial	12 mth/year					✓	Sulphation wind
62	Turner Valley	AIAAM	Industrial	3 mth/year					✓	Sulphation H_2S wind

NAPS - National Atmospheric Pollution Surveillance

AIAAM - Alberta Industry Ambient Air Monitoring

Table 19. Concluded

Station Name and Number	Location	Operated By	Type	Operation/ Frequency	Parameters Monitored: Oxidants O_3	NO_x	Particulate	CO	SO_2	Other
EIMU 90121	105 Ave and 17 Street	NAPS	Industrial		✓	✓	✓	✓	✓	Soiling Index Dustfall Sulphation HC
ERMU 90122	13335-127 Street	NAPS	Residential		✓	✓	✓	✓	✓	Soiling Index Dustfall Sulphation, HC
EDMU 90130	10255-104 Street	NAPS	Downtown		✓	✓	✓	✓	✓	Soiling Index HC Dustfall Sulphation AE
2	St. Albert	AIAAM	Industrial	12 mth/year >95% data availablity		✓			✓	H_2S Wind Sulphation
7	Redwater	AIAAM	Industrial	2 mth/year*					✓	H_2S Sulphation
8	Duhamel	AIAAM	Industrial	2 mth/year June/July					✓	H_2S Sulphation
9	Duhamel (Bittern Lake)	AIAAM	Industrial	2 mth/year					✓	H_2S Sulphation
16A	Clover Bar Forest Height	AIAAM	Industrial	12 mth/year		✓		✓	✓	
16B	102 Ave and 50 Street - Clover Bar Kennedale	AIAAM	Industrial	12 mth/year	✓	✓		✓		
17	Keephill's Wagners	AIAAM	Industrial	12 mth/year		✓	✓		✓	Sulphation Dustfall Wind
18A	Blacks	AIAAM	Industrial	12 mth/year		✓	✓		✓	Sulphation Dustfall Wind
18B	Kendricks	AIAAM	Industrial	12 mth/year		✓	✓		✓	Sulphation Dustfall Wind
18C	Melnyk	AIAAM	Industrial	12 mth/year		✓	✓		✓	Sulphation Dustfall Wind
19	Powers	AIAAM	Industrial	12 mth/year		✓	✓		✓	Sulphation Dustfall Wind
25A	Elmjay	AIAAM	Industrial	12 mth/year		✓				Wind Sulphation
25B	Goldbar	AIAAM	Industrial	12 mth/year					✓	H_2S Sulphation Wind
25C	Sherwood Park	AIAAM	Industrial	12 mth/year					✓	Sulphation, HC, H_2S
25D	Clover Bar	AIAAM	Industrial	12 mth/year	✓					Sulphation H_2S Wind
25E	Beverly	AIAAM	Industrial	12 mth/year		✓			✓	H_2S Sulphation HC Wind
25F	Clareview	AIAAM	Industrial	12 mth/year		✓			✓	Sulphation H_2S Wind

NAPS - National Atmospheric Pollution Surveillance

AIAAM - Alberta Industry Ambient Air Monitoring

5.7 SUMMARY

The data and hardware requirements of the Urban Airshed Model have been summarised, and have been compared with the data actually available for Edmonton and Calgary. It appears that the currently available data are nearly adequate to exercise the model using its minimum input options. However, to obtain credible model results, substantial data collection exercises will be required.

6. MODELS ON OTHER SPATIAL SCALES

Although the main thrust of this report was to identify the most appropriate urban-scale model for implementation in Alberta, together with its operational requirements, consideration was also given to those models applicable to the effects of urban pollution on other scales. Specifically included were effects occurring at, or due to, individual streets (street canyon and highway models) and effects of the urban plume on downwind points. Relative to modelling of the urban airshed as a whole, much less effort has been devoted to the development of models for these smaller and larger spatial scales. A brief review of currently available models is presented below.

6.1 HIGHWAY AND STREET CANYON MODELS

The physical and emission characteristics of highways and major urban streets (street canyons) are sufficiently different from those of the urban airshed that accurate prediction of pollutant concentrations in these areas requires special treatment. For example, street canyons are known to be somewhat isolated from upper air flow, and the recirculation (standing vortex) of the street canyon flow may trap pollution from automobile exhausts for extended periods of time. In general, calculation of the dispersion of atmospheric contaminants released from automobile exhausts at street level must include the effects of local geometry of buildings and trees bounding the street or highway, local topography, and climatological factors of wind speed, wind direction, and, to a lesser extent, temperature stratification.

The importance of understanding the above effects is well recognized, and many investigators have studied the problem experimentally in the field (e.g., Sobottka 1980; Wanner et al. 1977), or wind tunnels (e.g., Wedding et al. 1977). Because of the difficulty in parametrizing all of the physics, very few theoretical methods have been developed for predicting pollutant concentrations in street canyons.

Some of the simpler models are those presented by Ludwig and Debbert (1972), Wanner et al. (1977), and Sheih and Heilman (1978). Each of these is an analytical model. Ludwig and Dabbert used Gaussian theory and the others used simplified physical and dimensional arguments to derive their expressions for pollutant concentrations. None of the models account for wind direction.

These models were were not specifically developed for use as submodels in an urban airshed model, and to implement them would require resolution of some basic incompatibilities among the models. For example, a consistent means of relating the concentration in the street canyon to the source term in the airshed model must be developed. Also, the model of Sheih and Heilman must be extended to a third dimension (it is currently two dimensional) if it is to be used.

A final model that was considered for street canyons is that of Kotake and Sano (1981). This model is much more complete than the other models, as it incorporates all the relevant physics of the problem through the numerical solution of the three-dimensional Navier-Stokes and mass conservation equations at the subgrid level. Also calculated at the subgrid level is the reactive chemistry.

By solving the Navier-Stokes equations, no assumptions need to be made on the behaviour of the wind in the geometrically complicated configuration typical of urban areas. Consistency between the subgrid model (street canyon) and the airshed model would be achieved by using the result of the airshed model as boundary conditions for the street canyon model.

This model, while being complex and costly in terms of its computational requirements, would be useful as it would allow the effects of the geometrical configuration of streets and the nonlinear diffusion behaviour of chemically reactive pollutants to be examined. Also, the details of local air pollution at specified points could be investigated.

A model that was developed specifically for application to highways is the EPA HIWAY model (Zimmerman and Thompson, 1975). This

model uses Gaussian theory to calculate air quality levels of non-reactive pollutants in relatively uncomplicated terrain.

To date, no relatively simple yet acceptable method has been developed for predicting pollutant concentrations inside street canyons. To solve the problem, either very restrictive assumptions must be made, thus limiting the applicability of the model, or very complex, three-dimensional numerical techniques must be used that increase the already demanding computational requirements of the airshed model. The incorporation of this latter method could perhaps only be justified in major urban areas where traffic congestion is a severe problem. The lack of an appropriate street canyon submodel is an indication that further work is required in this area. While one of these models could be incorporated in the UAM, it is recommended that until sufficient need is shown for these models in the major urban centres of Alberta, one should not be chosen and implemented.

6.2 URBAN PLUME MODELS

There are at least three possible approaches to modelling the pollutant concentrations generated in the plume of an urban area:

1. Increase the domain size of the UAM,
2. Apply a simple Lagrangian scheme, or
3. Apply a sophisticated Lagrangian scheme.

These possibilities are discussed separately below.

If impacts relatively close to the urban area are to be considered, the first method may prove to be the most cost effective, since implementation of a second model would not be required. The domain of the UAM would simply be extended to include the point or points of interest. For distances of the order of 20 or 30 km this could be done in the course of modelling air quality in the urban airshed itself.

For greater downwind distances, computational economies could be achieved by performing a second run of the UAM using a coarser grid scale (e.g., 10 km). This run could make use of the airshed simulation as a source of initial conditions.

If economy of operation is an important consideration, as is the case when a large number of model runs will be required, the most satisfactory solution might be to make use of a simple Lagrangian formulation. Such a model has been described by Balko and Peters (1983). It considers a well-mixed parcel of air, originally located over the urban area, which is then advected by the mean wind, although it may be constrained to follow a previously determined trajectory. Chemical reactions occur within this parcel, which may be permitted to expand laterally, following a Gaussian prescription. The vertical extent of the air parcel is determined by the mixing depth.

Where marked inhomogeneities of emission rates are found, it will probably be necessary to use a more sophisticated Lagrangian formulation, such as PLMSTAR or ELSTAR (Lloyd et al. 1979). These models, which are basically similar, use a "wall of cells" approach, which provides spatial resolution in the cross wind direction. They both incorporate full photochemical mechanisms.

For longer distances (50 km or more), MESOPUFF2 has been found to possess greater technical strength than other Lagrangian models (CSC 1985).

Which of these approaches is the most appropriate for application to urban centres in Alberta is difficult to determine at present. It is recommended that specific details of the intended applications be delineated more clearly before a decision is made. It is worth noting, though, that the implementation costs of the first two approaches are much lower than that of the third.

7. CONCLUSIONS

The conclusions of this study are as follows:

1. A survey of user requirements revealed that these will best be met by a model of the Eulerian type, which includes a full photochemical mechanism.
2. A detailed theoretical evaluation of such models produced the conclusion that the Urban Airshed Model is the most suitable for implementation for the Alberta situation. The UAM possesses the following attributes:
   - i) It maintains a balance between computational economy and accurate representation of all relevant physics.
   - ii) It uses parametrizations close to state-of-the-art. When state-of-the-art is not used, UAM's modular design makes updating or replacement very easy to do. It also shows a good balance between its components.
   - iii) It provides a great deal of user flexibility. The formulation of the model (time-varying grid spacing and vertically varying vertical diffusivity), allows many different scenarios to be simulated (GENERALITY). Further, a choice of methods (interpolation, extrapolation, etc. of input data) allows it to be used with very little support data. This allows the user to acquire the model and run, for example, simplifed test problems immediately. There is not an immediate need to compile an extensive emissions inventory or set up an observational network.
   - iv) It will satisfy the needs of Alberta Environment (as specified in the Request for Proposal).
   - v) The model has been both verified (scientifically scrutinized) and validated (accepted and used by many different groups) and can therefore be used with confidence.

3. In contrast to urban airshed modelling, the state of modelling on smaller and larger spatial scales is less well developed. Fewer models are available. However, they cover a wide range of degrees of sophistication.
4. Limited input data are currently available for Edmonton and Calgary. Because the UAM has a minimum input option, these data are almost adequate to allow some model runs to be performed. However, only limited confidence can be placed in the results that will be produced. Further data collection is required.

8. RECOMMENDATIONS

The following recommendations result from the work described in the preceding sections of this report:

1. The Urban Airshed Model should be implemented for application to the study of air quality in urban centres in Alberta. It should be cautioned that all models of this type are very sophisticated computer codes, and credible results can only be obtained if the team running the model has a detailed understanding of the workings of the code and of its data requirements. To illustrate this, the Association of Bay Area Governments (1979) recommended that the team include personnel with experience and expertise in atmospheric chemistry, dynamic meteorology/turbulent flow and transport, numerical methods, and computer science.
2. The model should be exercised using its minimum input options to allow experience to be gained in its operation.
3. Plans should be prepared for programs that will provide the input and validation data necessary for the production of credible model predictions. These would include:
   i) Further manipulation of the Calgary and Edmonton emission inventories to provide the required chemical and temporal resolution, plus supplementation of the data (if this is required to cover the entire model domain);
   ii) Supplementation of existing networks to improve the data coverage for initial and boundary conditions, wind field, etc. (upper air data are particularly required); and
   iii) Intensive short-term studies, preferably coinciding with pollution episodes, to provide model validation data.

4. The wind field generator required by the model has been regarded as a separate, site-specific item, and a suitable generator was not identified in the present study. This component must be specified for future use.
5. Consideration should be given to the incorporation of refinements to the model:
   i) A definite requirement is that the most up-to-date version of CBM be installed, including the improvements discussed in Section 3.
   ii) The introduction of modified upwind difference methods will reduce the amount of false diffusion introduced by the transport algorithm.
   iii) The use of implicit formulations and vectorization of the code should result in significant reductions in computational effort.

No recommendations regarding street canyon, highway, or regional-scale models have been made at this time. Detailed recommendations regarding data collection for operation of the model have not been given. Since the model allows a range of input options, it will be most appropriate to prepare a staged set of plans for measurement programs, together with an estimate of the cost of undertaking each. The stages would range from using existing data to making measurements of meteorological and atmospheric parameters (e.g., wind speed and direction, inversion height, temperature, pressure, and relative humidity) and chemical species concentrations (all emitted species plus ozone, PAN, HNO_3, etc.) at as many points as possible (e.g., up to 10 or more) within the urban area.

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